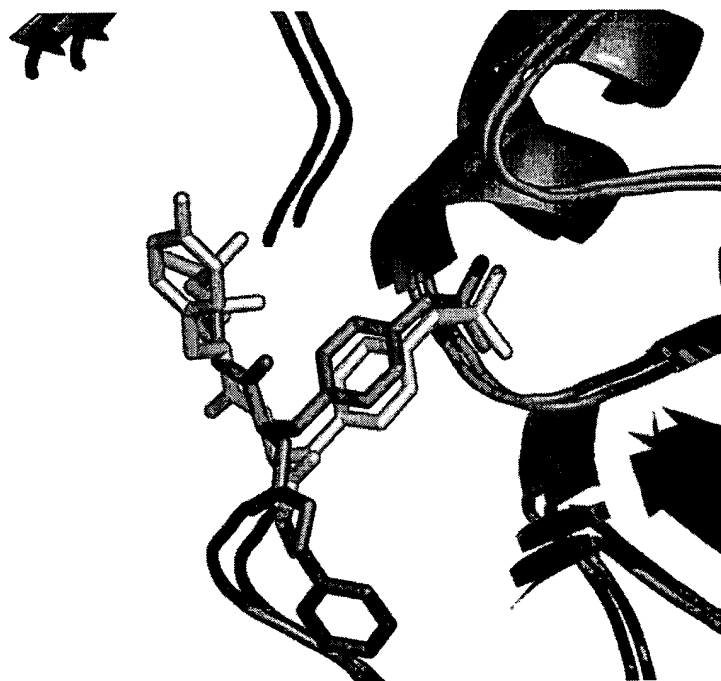


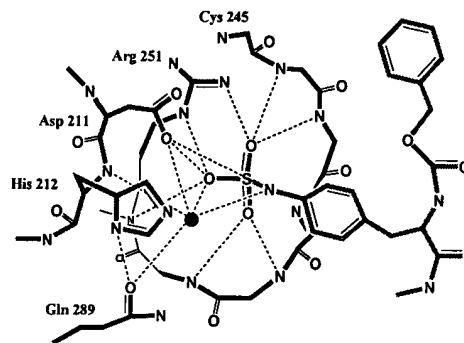
**FIGURE 1**



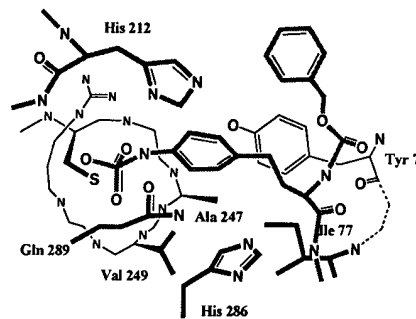
**FIGURE 2**



**FIGURE 3**



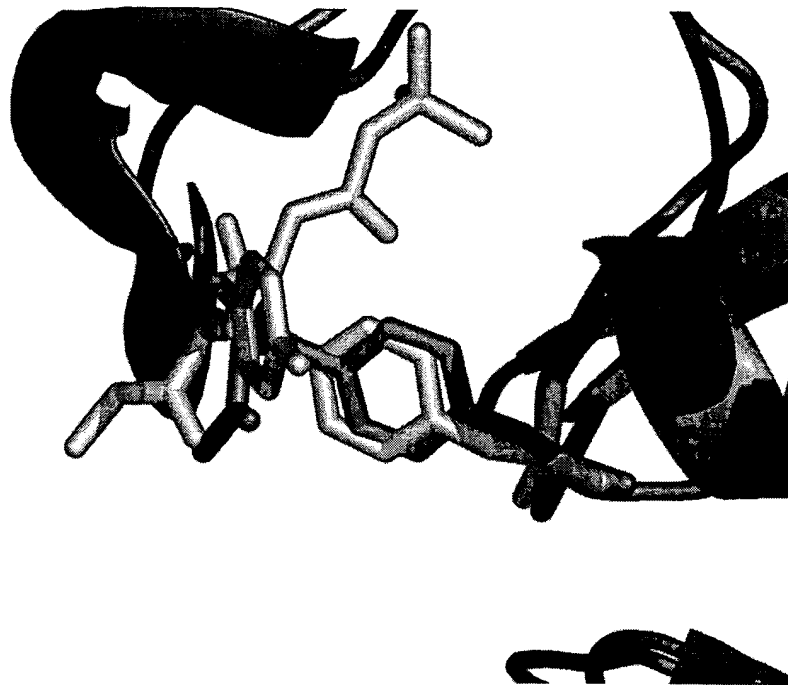
(a)



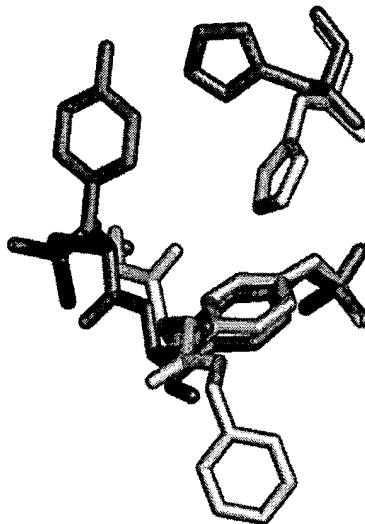
(b)

FIGURE 4





**FIGURE 5**



**FIGURE 6**

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Three Dimensional Coordinates of HPTPbeta

|        |        |        |          |        |        |        |             |
|--------|--------|--------|----------|--------|--------|--------|-------------|
| CRYST1 | 61.890 | 71.535 | 70.345   | 90.00  | 93.25  | 90.00  |             |
| ATOM   | 1      | N      | LYS A 19 | 12.885 | 20.303 | 21.460 | 1.000106.97 |
| ATOM   | 2      | CA     | LYS A 19 | 12.939 | 19.537 | 20.223 | 1.000 85.75 |
| ATOM   | 3      | CB     | LYS A 19 | 13.192 | 20.422 | 19.007 | 1.000 87.72 |
| ATOM   | 4      | CG     | LYS A 19 | 11.902 | 20.923 | 18.320 | 1.000 95.27 |
| ATOM   | 5      | CD     | LYS A 19 | 12.014 | 20.782 | 16.801 | 1.000 99.48 |
| ATOM   | 6      | CE     | LYS A 19 | 10.663 | 21.012 | 16.143 | 1.000100.17 |
| ATOM   | 7      | NZ     | LYS A 19 | 10.303 | 22.523 | 16.035 | 1.000102.13 |
| ATOM   | 8      | C      | LYS A 19 | 14.027 | 18.457 | 20.298 | 1.000 78.84 |
| ATOM   | 9      | O      | LYS A 19 | 15.217 | 18.783 | 20.327 | 1.000 93.11 |
| ATOM   | 10     | N      | THR A 20 | 13.573 | 17.224 | 20.310 | 1.000 69.90 |
| ATOM   | 11     | CA     | THR A 20 | 14.257 | 15.957 | 20.169 | 1.000 59.58 |
| ATOM   | 12     | CB     | THR A 20 | 13.713 | 15.258 | 18.900 | 1.000 45.21 |
| ATOM   | 13     | OG1    | THR A 20 | 14.633 | 14.309 | 18.358 | 1.000 57.38 |
| ATOM   | 14     | CG2    | THR A 20 | 13.489 | 16.286 | 17.795 | 1.000 64.36 |
| ATOM   | 15     | C      | THR A 20 | 15.771 | 16.101 | 20.107 | 1.000 59.34 |
| ATOM   | 16     | O      | THR A 20 | 16.304 | 16.833 | 19.272 | 1.000 83.31 |
| ATOM   | 17     | N      | SER A 21 | 16.471 | 15.408 | 20.994 | 1.000 53.48 |
| ATOM   | 18     | CA     | SER A 21 | 17.903 | 15.206 | 20.988 | 1.000 46.96 |
| ATOM   | 19     | CB     | SER A 21 | 18.353 | 14.742 | 19.581 | 1.000 47.66 |
| ATOM   | 20     | OG     | SER A 21 | 19.770 | 14.620 | 19.599 | 1.000 58.97 |
| ATOM   | 21     | C      | SER A 21 | 18.784 | 16.398 | 21.346 | 1.000 41.17 |
| ATOM   | 22     | O      | SER A 21 | 18.538 | 17.534 | 20.963 | 1.000 47.65 |
| ATOM   | 23     | N      | CYS A 22 | 19.843 | 16.085 | 22.080 | 1.000 41.72 |
| ATOM   | 24     | CA     | CYS A 22 | 20.898 | 16.977 | 22.509 | 1.000 43.91 |
| ATOM   | 25     | CB     | CYS A 22 | 20.566 | 17.726 | 23.798 | 1.000 41.39 |
| ATOM   | 26     | SG     | CYS A 22 | 19.635 | 19.259 | 23.584 | 1.000109.59 |
| ATOM   | 27     | C      | CYS A 22 | 22.183 | 16.174 | 22.752 | 1.000 37.65 |
| ATOM   | 28     | O      | CYS A 22 | 22.505 | 15.999 | 23.925 | 1.000 36.88 |
| ATOM   | 29     | N      | PRO A 23 | 22.822 | 15.731 | 21.680 | 1.000 42.64 |
| ATOM   | 30     | CA     | PRO A 23 | 24.007 | 14.873 | 21.736 | 1.000 46.23 |
| ATOM   | 31     | CB     | PRO A 23 | 24.238 | 14.461 | 20.277 | 1.000 45.02 |
| ATOM   | 32     | CG     | PRO A 23 | 23.012 | 14.867 | 19.533 | 1.000 44.64 |
| ATOM   | 33     | CD     | PRO A 23 | 22.447 | 16.037 | 20.280 | 1.000 45.34 |
| ATOM   | 34     | C      | PRO A 23 | 25.254 | 15.595 | 22.253 | 1.000 49.52 |
| ATOM   | 35     | O      | PRO A 23 | 25.409 | 16.802 | 22.079 | 1.000 43.06 |
| ATOM   | 36     | N      | ILE A 24 | 26.145 | 14.847 | 22.897 | 1.000 50.39 |
| ATOM   | 37     | CA     | ILE A 24 | 27.396 | 15.350 | 23.436 | 1.000 45.58 |
| ATOM   | 38     | CB     | ILE A 24 | 27.299 | 15.718 | 24.926 | 1.000 45.32 |
| ATOM   | 39     | CG1    | ILE A 24 | 26.035 | 16.480 | 25.330 | 1.000 43.71 |
| ATOM   | 40     | CD1    | ILE A 24 | 25.222 | 15.741 | 26.376 | 1.000 43.61 |
| ATOM   | 41     | CG2    | ILE A 24 | 28.545 | 16.488 | 25.350 | 1.000 57.16 |
| ATOM   | 42     | C      | ILE A 24 | 28.517 | 14.327 | 23.296 | 1.000 43.32 |
| ATOM   | 43     | O      | ILE A 24 | 28.322 | 13.140 | 23.537 | 1.000 46.87 |
| ATOM   | 44     | N      | LYS A 25 | 29.713 | 14.766 | 22.907 | 1.000 49.84 |
| ATOM   | 45     | CA     | LYS A 25 | 30.820 | 13.808 | 22.815 | 1.000 50.13 |
| ATOM   | 46     | CB     | LYS A 25 | 31.917 | 14.375 | 21.922 | 1.000 59.09 |
| ATOM   | 47     | CG     | LYS A 25 | 31.444 | 14.757 | 20.527 | 1.000 65.03 |
| ATOM   | 48     | CD     | LYS A 25 | 32.307 | 14.074 | 19.471 | 1.000 71.18 |
| ATOM   | 49     | CE     | LYS A 25 | 31.469 | 13.255 | 18.493 | 1.000 72.46 |
| ATOM   | 50     | NZ     | LYS A 25 | 32.328 | 12.452 | 17.576 | 1.000 73.47 |
| ATOM   | 51     | C      | LYS A 25 | 31.346 | 13.486 | 24.204 | 1.000 52.08 |

**FIGURE 7**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 52  | O   | LYS | A | 25 | 31.294 | 14.340 | 25.095 | 1.000 | 53.68 |
| ATOM | 53  | N   | ILE | A | 26 | 31.849 | 12.274 | 24.434 | 1.000 | 52.14 |
| ATOM | 54  | CA  | ILE | A | 26 | 32.275 | 11.942 | 25.793 | 1.000 | 63.74 |
| ATOM | 55  | CB  | ILE | A | 26 | 32.817 | 10.504 | 25.904 | 1.000 | 65.16 |
| ATOM | 56  | CG1 | ILE | A | 26 | 34.316 | 10.370 | 25.624 | 1.000 | 65.92 |
| ATOM | 57  | CD1 | ILE | A | 26 | 34.847 | 8.970  | 25.852 | 1.000 | 69.50 |
| ATOM | 58  | CG2 | ILE | A | 26 | 32.016 | 9.561  | 25.016 | 1.000 | 68.17 |
| ATOM | 59  | C   | ILE | A | 26 | 33.335 | 12.911 | 26.307 | 1.000 | 70.34 |
| ATOM | 60  | O   | ILE | A | 26 | 33.411 | 13.146 | 27.515 | 1.000 | 67.42 |
| ATOM | 61  | N   | ASN | A | 27 | 34.141 | 13.465 | 25.406 | 1.000 | 74.12 |
| ATOM | 62  | CA  | ASN | A | 27 | 35.231 | 14.350 | 25.799 | 1.000 | 78.44 |
| ATOM | 63  | CB  | ASN | A | 27 | 36.116 | 14.679 | 24.588 | 1.000 | 86.40 |
| ATOM | 64  | CG  | ASN | A | 27 | 36.877 | 15.980 | 24.768 | 1.000 | 90.22 |
| ATOM | 65  | OD1 | ASN | A | 27 | 37.854 | 16.044 | 25.515 | 1.000 | 84.42 |
| ATOM | 66  | ND2 | ASN | A | 27 | 36.432 | 17.033 | 24.084 | 1.000 | 85.29 |
| ATOM | 67  | C   | ASN | A | 27 | 34.740 | 15.649 | 26.423 | 1.000 | 75.19 |
| ATOM | 68  | O   | ASN | A | 27 | 35.473 | 16.309 | 27.170 | 1.000 | 89.55 |
| ATOM | 69  | N   | GLN | A | 28 | 33.507 | 16.048 | 26.126 | 1.000 | 67.31 |
| ATOM | 70  | CA  | GLN | A | 28 | 33.008 | 17.350 | 26.550 | 1.000 | 57.01 |
| ATOM | 71  | CB  | GLN | A | 28 | 32.497 | 18.097 | 25.313 | 1.000 | 54.35 |
| ATOM | 72  | CG  | GLN | A | 28 | 32.204 | 19.571 | 25.517 | 1.000 | 59.01 |
| ATOM | 73  | CD  | GLN | A | 28 | 32.233 | 20.351 | 24.213 | 1.000 | 66.07 |
| ATOM | 74  | OE1 | GLN | A | 28 | 31.315 | 21.121 | 23.907 | 1.000 | 69.78 |
| ATOM | 75  | NE2 | GLN | A | 28 | 33.291 | 20.154 | 23.427 | 1.000 | 81.02 |
| ATOM | 76  | C   | GLN | A | 28 | 31.894 | 17.263 | 27.581 | 1.000 | 51.77 |
| ATOM | 77  | O   | GLN | A | 28 | 31.322 | 18.300 | 27.939 | 1.000 | 55.71 |
| ATOM | 78  | N   | PHE | A | 29 | 31.566 | 16.061 | 28.051 | 1.000 | 50.17 |
| ATOM | 79  | CA  | PHE | A | 29 | 30.395 | 15.896 | 28.910 | 1.000 | 48.12 |
| ATOM | 80  | CB  | PHE | A | 29 | 29.984 | 14.424 | 29.031 | 1.000 | 47.45 |
| ATOM | 81  | CG  | PHE | A | 29 | 28.679 | 14.209 | 29.760 | 1.000 | 51.71 |
| ATOM | 82  | CD1 | PHE | A | 29 | 27.473 | 14.198 | 29.076 | 1.000 | 47.01 |
| ATOM | 83  | CE1 | PHE | A | 29 | 26.272 | 14.005 | 29.732 | 1.000 | 44.54 |
| ATOM | 84  | CZ  | PHE | A | 29 | 26.254 | 13.826 | 31.104 | 1.000 | 53.70 |
| ATOM | 85  | CE2 | PHE | A | 29 | 27.448 | 13.826 | 31.808 | 1.000 | 58.73 |
| ATOM | 86  | CD2 | PHE | A | 29 | 28.641 | 14.016 | 31.134 | 1.000 | 58.31 |
| ATOM | 87  | C   | PHE | A | 29 | 30.633 | 16.505 | 30.293 | 1.000 | 48.21 |
| ATOM | 88  | O   | PHE | A | 29 | 29.805 | 17.313 | 30.723 | 1.000 | 51.21 |
| ATOM | 89  | N   | GLU | A | 30 | 31.725 | 16.100 | 30.932 | 1.000 | 50.97 |
| ATOM | 90  | CA  | GLU | A | 30 | 32.118 | 16.617 | 32.243 | 1.000 | 40.77 |
| ATOM | 91  | CB  | GLU | A | 30 | 33.518 | 16.157 | 32.627 | 1.000 | 48.14 |
| ATOM | 92  | CG  | GLU | A | 30 | 33.957 | 16.520 | 34.038 | 1.000 | 61.37 |
| ATOM | 93  | CD  | GLU | A | 30 | 34.375 | 15.319 | 34.871 | 1.000 | 63.56 |
| ATOM | 94  | OE1 | GLU | A | 30 | 34.907 | 14.350 | 34.287 | 1.000 | 58.37 |
| ATOM | 95  | OE2 | GLU | A | 30 | 34.180 | 15.327 | 36.108 | 1.000 | 52.10 |
| ATOM | 96  | C   | GLU | A | 30 | 32.029 | 18.136 | 32.196 | 1.000 | 42.41 |
| ATOM | 97  | O   | GLU | A | 30 | 31.394 | 18.780 | 33.026 | 1.000 | 53.55 |
| ATOM | 98  | N   | GLY | A | 31 | 32.650 | 18.719 | 31.167 | 1.000 | 41.84 |
| ATOM | 99  | CA  | GLY | A | 31 | 32.510 | 20.160 | 31.001 | 1.000 | 40.41 |
| ATOM | 100 | C   | GLY | A | 31 | 31.063 | 20.531 | 30.754 | 1.000 | 48.99 |
| ATOM | 101 | O   | GLY | A | 31 | 30.515 | 21.443 | 31.373 | 1.000 | 50.79 |
| ATOM | 102 | N   | HIS | A | 32 | 30.407 | 19.821 | 29.826 | 1.000 | 45.73 |
| ATOM | 103 | CA  | HIS | A | 32 | 29.036 | 20.224 | 29.519 | 1.000 | 40.05 |

**FIGURE 8**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |        |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 104 | CB  | HIS | A | 32 | 28.481 | 19.370 | 28.368 | 1.000 | 44.33  |
| ATOM | 105 | CG  | HIS | A | 32 | 26.991 | 19.509 | 28.268 | 1.000 | 46.74  |
| ATOM | 106 | ND1 | HIS | A | 32 | 26.393 | 20.629 | 27.736 | 1.000 | 49.67  |
| ATOM | 107 | CE1 | HIS | A | 32 | 25.081 | 20.489 | 27.779 | 1.000 | 47.50  |
| ATOM | 108 | NE2 | HIS | A | 32 | 24.803 | 19.318 | 28.328 | 1.000 | 46.49  |
| ATOM | 109 | CD2 | HIS | A | 32 | 25.985 | 18.688 | 28.642 | 1.000 | 48.61  |
| ATOM | 110 | C   | HIS | A | 32 | 28.128 | 20.126 | 30.738 | 1.000 | 36.48  |
| ATOM | 111 | O   | HIS | A | 32 | 27.213 | 20.935 | 30.894 | 1.000 | 47.25  |
| ATOM | 112 | N   | PHE | A | 33 | 28.355 | 19.146 | 31.611 | 1.000 | 37.04  |
| ATOM | 113 | CA  | PHE | A | 33 | 27.466 | 18.940 | 32.760 | 1.000 | 45.61  |
| ATOM | 114 | CB  | PHE | A | 33 | 27.679 | 17.531 | 33.322 | 1.000 | 44.57  |
| ATOM | 115 | CG  | PHE | A | 33 | 26.836 | 17.160 | 34.514 | 1.000 | 38.23  |
| ATOM | 116 | CD1 | PHE | A | 33 | 25.506 | 17.531 | 34.598 | 1.000 | 30.80  |
| ATOM | 117 | CE1 | PHE | A | 33 | 24.748 | 17.191 | 35.702 | 1.000 | 28.41  |
| ATOM | 118 | CZ  | PHE | A | 33 | 25.308 | 16.468 | 36.737 | 1.000 | 30.68  |
| ATOM | 119 | CE2 | PHE | A | 33 | 26.635 | 16.088 | 36.669 | 1.000 | 27.11  |
| ATOM | 120 | CD2 | PHE | A | 33 | 27.378 | 16.436 | 35.564 | 1.000 | 28.82  |
| ATOM | 121 | C   | PHE | A | 33 | 27.652 | 19.998 | 33.837 | 1.000 | 49.01  |
| ATOM | 122 | O   | PHE | A | 33 | 26.723 | 20.391 | 34.548 | 1.000 | 35.78  |
| ATOM | 123 | N   | MET | A | 34 | 28.873 | 20.503 | 33.990 | 1.000 | 55.36  |
| ATOM | 124 | CA  | MET | A | 34 | 29.145 | 21.595 | 34.918 | 1.000 | 48.73  |
| ATOM | 125 | CB  | MET | A | 34 | 30.612 | 22.002 | 34.804 | 1.000 | 50.55  |
| ATOM | 126 | CG  | MET | A | 34 | 31.589 | 20.956 | 35.319 | 1.000 | 44.00  |
| ATOM | 127 | SD  | MET | A | 34 | 31.900 | 21.178 | 37.082 | 1.000 | 69.37  |
| ATOM | 128 | CE  | MET | A | 34 | 32.522 | 19.553 | 37.528 | 1.000 | 157.91 |
| ATOM | 129 | C   | MET | A | 34 | 28.257 | 22.797 | 34.629 | 1.000 | 45.46  |
| ATOM | 130 | O   | MET | A | 34 | 27.672 | 23.409 | 35.524 | 1.000 | 51.08  |
| ATOM | 131 | N   | LYS | A | 35 | 28.169 | 23.133 | 33.343 | 1.000 | 42.34  |
| ATOM | 132 | CA  | LYS | A | 35 | 27.337 | 24.249 | 32.905 | 1.000 | 41.76  |
| ATOM | 133 | CB  | LYS | A | 35 | 27.357 | 24.341 | 31.387 | 1.000 | 48.16  |
| ATOM | 134 | CG  | LYS | A | 35 | 28.744 | 24.409 | 30.774 | 1.000 | 54.19  |
| ATOM | 135 | CD  | LYS | A | 35 | 28.745 | 25.343 | 29.558 | 1.000 | 56.45  |
| ATOM | 136 | CE  | LYS | A | 35 | 27.969 | 26.621 | 29.849 | 1.000 | 59.03  |
| ATOM | 137 | NZ  | LYS | A | 35 | 26.532 | 26.499 | 29.466 | 1.000 | 63.17  |
| ATOM | 138 | C   | LYS | A | 35 | 25.902 | 24.093 | 33.401 | 1.000 | 52.49  |
| ATOM | 139 | O   | LYS | A | 35 | 25.341 | 25.000 | 34.019 | 1.000 | 58.86  |
| ATOM | 140 | N   | LEU | A | 36 | 25.323 | 22.927 | 33.122 | 1.000 | 45.81  |
| ATOM | 141 | CA  | LEU | A | 36 | 23.967 | 22.608 | 33.538 | 1.000 | 38.58  |
| ATOM | 142 | CB  | LEU | A | 36 | 23.651 | 21.126 | 33.313 | 1.000 | 45.57  |
| ATOM | 143 | CG  | LEU | A | 36 | 23.288 | 20.682 | 31.901 | 1.000 | 50.85  |
| ATOM | 144 | CD1 | LEU | A | 36 | 24.233 | 21.277 | 30.870 | 1.000 | 57.32  |
| ATOM | 145 | CD2 | LEU | A | 36 | 23.292 | 19.159 | 31.799 | 1.000 | 59.71  |
| ATOM | 146 | C   | LEU | A | 36 | 23.753 | 22.921 | 35.011 | 1.000 | 35.30  |
| ATOM | 147 | O   | LEU | A | 36 | 22.857 | 23.679 | 35.382 | 1.000 | 53.13  |
| ATOM | 148 | N   | GLN | A | 37 | 24.585 | 22.311 | 35.857 | 1.000 | 36.39  |
| ATOM | 149 | CA  | GLN | A | 37 | 24.427 | 22.527 | 37.292 | 1.000 | 46.18  |
| ATOM | 150 | CB  | GLN | A | 37 | 25.238 | 21.504 | 38.085 | 1.000 | 56.71  |
| ATOM | 151 | CG  | GLN | A | 37 | 26.311 | 20.782 | 37.289 | 1.000 | 59.65  |
| ATOM | 152 | CD  | GLN | A | 37 | 26.681 | 19.440 | 37.891 | 1.000 | 59.86  |
| ATOM | 153 | OE1 | GLN | A | 37 | 27.412 | 18.655 | 37.285 | 1.000 | 76.78  |
| ATOM | 154 | NE2 | GLN | A | 37 | 26.190 | 19.165 | 39.092 | 1.000 | 59.17  |
| ATOM | 155 | C   | GLN | A | 37 | 24.844 | 23.938 | 37.696 | 1.000 | 53.32  |

**FIGURE 9**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |        |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 156 | O   | GLN | A | 37 | 24.407 | 24.448 | 38.730 | 1.000 | 47.35  |
| ATOM | 157 | N   | ALA | A | 38 | 25.684 | 24.560 | 36.876 | 1.000 | 58.65  |
| ATOM | 158 | CA  | ALA | A | 38 | 26.173 | 25.905 | 37.151 | 1.000 | 68.20  |
| ATOM | 159 | CB  | ALA | A | 38 | 27.038 | 26.387 | 35.992 | 1.000 | 88.29  |
| ATOM | 160 | C   | ALA | A | 38 | 25.055 | 26.906 | 37.416 | 1.000 | 68.67  |
| ATOM | 161 | O   | ALA | A | 38 | 24.003 | 26.933 | 36.777 | 1.000 | 57.74  |
| ATOM | 162 | N   | ASP | A | 39 | 25.301 | 27.778 | 38.394 | 1.000 | 72.20  |
| ATOM | 163 | CA  | ASP | A | 39 | 24.314 | 28.796 | 38.736 | 1.000 | 74.27  |
| ATOM | 164 | CB  | ASP | A | 39 | 23.909 | 29.628 | 37.527 | 1.000 | 85.74  |
| ATOM | 165 | CG  | ASP | A | 39 | 25.044 | 30.402 | 36.878 | 1.000 | 97.59  |
| ATOM | 166 | OD1 | ASP | A | 39 | 24.958 | 30.635 | 35.641 | 1.000 | 113.10 |
| ATOM | 167 | OD2 | ASP | A | 39 | 26.039 | 30.750 | 37.574 | 1.000 | 105.88 |
| ATOM | 168 | C   | ASP | A | 39 | 23.087 | 28.123 | 39.343 | 1.000 | 66.70  |
| ATOM | 169 | O   | ASP | A | 39 | 21.999 | 28.689 | 39.281 | 1.000 | 73.27  |
| ATOM | 170 | N   | SER | A | 40 | 23.298 | 26.947 | 39.907 | 1.000 | 64.44  |
| ATOM | 171 | CA  | SER | A | 40 | 22.275 | 26.159 | 40.578 | 1.000 | 64.68  |
| ATOM | 172 | CB  | SER | A | 40 | 21.396 | 27.050 | 41.465 | 1.000 | 55.65  |
| ATOM | 173 | OG  | SER | A | 40 | 22.105 | 28.171 | 41.962 | 1.000 | 78.01  |
| ATOM | 174 | C   | SER | A | 40 | 21.376 | 25.400 | 39.603 | 1.000 | 62.90  |
| ATOM | 175 | O   | SER | A | 40 | 20.184 | 25.716 | 39.507 | 1.000 | 51.42  |
| ATOM | 176 | N   | ASN | A | 41 | 21.912 | 24.422 | 38.883 | 1.000 | 60.85  |
| ATOM | 177 | CA  | ASN | A | 41 | 21.172 | 23.654 | 37.894 | 1.000 | 61.49  |
| ATOM | 178 | CB  | ASN | A | 41 | 20.165 | 22.694 | 38.532 | 1.000 | 61.83  |
| ATOM | 179 | CG  | ASN | A | 41 | 20.762 | 21.620 | 39.402 | 1.000 | 69.08  |
| ATOM | 180 | OD1 | ASN | A | 41 | 21.917 | 21.225 | 39.250 | 1.000 | 80.40  |
| ATOM | 181 | ND2 | ASN | A | 41 | 19.957 | 21.130 | 40.339 | 1.000 | 78.07  |
| ATOM | 182 | C   | ASN | A | 41 | 20.361 | 24.555 | 36.966 | 1.000 | 67.15  |
| ATOM | 183 | O   | ASN | A | 41 | 19.289 | 24.130 | 36.528 | 1.000 | 80.59  |
| ATOM | 184 | N   | TYR | A | 42 | 20.825 | 25.767 | 36.685 | 1.000 | 63.68  |
| ATOM | 185 | CA  | TYR | A | 42 | 19.955 | 26.712 | 35.995 | 1.000 | 58.60  |
| ATOM | 186 | CB  | TYR | A | 42 | 20.581 | 28.109 | 35.929 | 1.000 | 62.78  |
| ATOM | 187 | CG  | TYR | A | 42 | 19.713 | 29.057 | 35.134 | 1.000 | 60.11  |
| ATOM | 188 | CD1 | TYR | A | 42 | 18.414 | 29.333 | 35.553 | 1.000 | 62.46  |
| ATOM | 189 | CE1 | TYR | A | 42 | 17.603 | 30.195 | 34.844 | 1.000 | 61.51  |
| ATOM | 190 | CZ  | TYR | A | 42 | 18.099 | 30.785 | 33.705 | 1.000 | 62.86  |
| ATOM | 191 | OH  | TYR | A | 42 | 17.300 | 31.648 | 32.990 | 1.000 | 84.83  |
| ATOM | 192 | CE2 | TYR | A | 42 | 19.378 | 30.523 | 33.263 | 1.000 | 60.46  |
| ATOM | 193 | CD2 | TYR | A | 42 | 20.186 | 29.658 | 33.976 | 1.000 | 59.75  |
| ATOM | 194 | C   | TYR | A | 42 | 19.631 | 26.234 | 34.584 | 1.000 | 44.43  |
| ATOM | 195 | O   | TYR | A | 42 | 18.468 | 26.109 | 34.216 | 1.000 | 44.77  |
| ATOM | 196 | N   | LEU | A | 43 | 20.701 | 25.982 | 33.847 | 1.000 | 40.94  |
| ATOM | 197 | CA  | LEU | A | 43 | 20.603 | 25.447 | 32.499 | 1.000 | 53.15  |
| ATOM | 198 | CB  | LEU | A | 43 | 21.973 | 25.359 | 31.837 | 1.000 | 60.19  |
| ATOM | 199 | CG  | LEU | A | 43 | 22.899 | 26.570 | 31.920 | 1.000 | 67.43  |
| ATOM | 200 | CD1 | LEU | A | 43 | 23.839 | 26.600 | 30.724 | 1.000 | 71.66  |
| ATOM | 201 | CD2 | LEU | A | 43 | 22.126 | 27.871 | 32.003 | 1.000 | 79.71  |
| ATOM | 202 | C   | LEU | A | 43 | 19.934 | 24.068 | 32.542 | 1.000 | 55.94  |
| ATOM | 203 | O   | LEU | A | 43 | 18.895 | 23.893 | 31.904 | 1.000 | 56.22  |
| ATOM | 204 | N   | LEU | A | 44 | 20.523 | 23.138 | 33.277 | 1.000 | 55.33  |
| ATOM | 205 | CA  | LEU | A | 44 | 20.043 | 21.785 | 33.466 | 1.000 | 57.43  |
| ATOM | 206 | CB  | LEU | A | 44 | 20.668 | 21.151 | 34.719 | 1.000 | 58.28  |
| ATOM | 207 | CG  | LEU | A | 44 | 20.333 | 19.672 | 34.935 | 1.000 | 58.45  |

**FIGURE 10**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 208 | CD1 | LEU | A | 44 | 21.583 | 18.890 | 35.306 | 1.000 | 66.34 |
| ATOM | 209 | CD2 | LEU | A | 44 | 19.259 | 19.509 | 35.999 | 1.000 | 64.52 |
| ATOM | 210 | C   | LEU | A | 44 | 18.522 | 21.721 | 33.618 | 1.000 | 58.45 |
| ATOM | 211 | O   | LEU | A | 44 | 17.875 | 20.876 | 33.005 | 1.000 | 62.57 |
| ATOM | 212 | N   | SER | A | 45 | 18.022 | 22.636 | 34.428 | 1.000 | 58.88 |
| ATOM | 213 | CA  | SER | A | 45 | 16.634 | 22.760 | 34.841 | 1.000 | 54.60 |
| ATOM | 214 | CB  | SER | A | 45 | 16.564 | 23.645 | 36.093 | 1.000 | 50.24 |
| ATOM | 215 | OG  | SER | A | 45 | 15.228 | 23.927 | 36.463 | 1.000 | 55.87 |
| ATOM | 216 | C   | SER | A | 45 | 15.745 | 23.315 | 33.743 | 1.000 | 57.32 |
| ATOM | 217 | O   | SER | A | 45 | 14.548 | 23.027 | 33.655 | 1.000 | 57.44 |
| ATOM | 218 | N   | LYS | A | 46 | 16.303 | 24.131 | 32.849 | 1.000 | 62.62 |
| ATOM | 219 | CA  | LYS | A | 46 | 15.432 | 24.625 | 31.776 | 1.000 | 66.95 |
| ATOM | 220 | CB  | LYS | A | 46 | 15.937 | 25.962 | 31.242 | 1.000 | 74.26 |
| ATOM | 221 | CG  | LYS | A | 46 | 16.359 | 26.942 | 32.327 | 1.000 | 76.81 |
| ATOM | 222 | CD  | LYS | A | 46 | 15.163 | 27.555 | 33.036 | 1.000 | 76.98 |
| ATOM | 223 | CE  | LYS | A | 46 | 13.919 | 27.533 | 32.159 | 1.000 | 77.01 |
| ATOM | 224 | NZ  | LYS | A | 46 | 13.910 | 28.669 | 31.183 | 1.000 | 76.61 |
| ATOM | 225 | C   | LYS | A | 46 | 15.324 | 23.574 | 30.673 | 1.000 | 58.56 |
| ATOM | 226 | O   | LYS | A | 46 | 14.244 | 23.378 | 30.116 | 1.000 | 75.22 |
| ATOM | 227 | N   | GLU | A | 47 | 16.436 | 22.917 | 30.384 | 1.000 | 47.55 |
| ATOM | 228 | CA  | GLU | A | 47 | 16.525 | 21.820 | 29.431 | 1.000 | 50.54 |
| ATOM | 229 | CB  | GLU | A | 47 | 17.934 | 21.229 | 29.416 | 1.000 | 51.00 |
| ATOM | 230 | CG  | GLU | A | 47 | 18.207 | 20.220 | 28.322 | 1.000 | 54.12 |
| ATOM | 231 | CD  | GLU | A | 47 | 19.602 | 19.627 | 28.395 | 1.000 | 52.91 |
| ATOM | 232 | OE1 | GLU | A | 47 | 20.500 | 20.053 | 27.631 | 1.000 | 41.94 |
| ATOM | 233 | OE2 | GLU | A | 47 | 19.799 | 18.714 | 29.229 | 1.000 | 49.31 |
| ATOM | 234 | C   | GLU | A | 47 | 15.509 | 20.738 | 29.790 | 1.000 | 49.73 |
| ATOM | 235 | O   | GLU | A | 47 | 14.803 | 20.208 | 28.939 | 1.000 | 39.85 |
| ATOM | 236 | N   | TYR | A | 48 | 15.448 | 20.426 | 31.086 | 1.000 | 44.02 |
| ATOM | 237 | CA  | TYR | A | 48 | 14.563 | 19.352 | 31.531 | 1.000 | 41.02 |
| ATOM | 238 | CB  | TYR | A | 48 | 14.890 | 18.965 | 32.971 | 1.000 | 38.64 |
| ATOM | 239 | CG  | TYR | A | 48 | 13.922 | 17.993 | 33.599 | 1.000 | 36.61 |
| ATOM | 240 | CD1 | TYR | A | 48 | 13.950 | 16.650 | 33.247 | 1.000 | 34.64 |
| ATOM | 241 | CE1 | TYR | A | 48 | 13.073 | 15.745 | 33.809 | 1.000 | 36.45 |
| ATOM | 242 | CZ  | TYR | A | 48 | 12.153 | 16.179 | 34.738 | 1.000 | 35.24 |
| ATOM | 243 | OH  | TYR | A | 48 | 11.285 | 15.269 | 35.288 | 1.000 | 36.83 |
| ATOM | 244 | CE2 | TYR | A | 48 | 12.098 | 17.506 | 35.108 | 1.000 | 34.92 |
| ATOM | 245 | CD2 | TYR | A | 48 | 12.983 | 18.405 | 34.535 | 1.000 | 38.27 |
| ATOM | 246 | C   | TYR | A | 48 | 13.112 | 19.774 | 31.382 | 1.000 | 42.44 |
| ATOM | 247 | O   | TYR | A | 48 | 12.227 | 18.943 | 31.170 | 1.000 | 37.58 |
| ATOM | 248 | N   | GLU | A | 49 | 12.839 | 21.077 | 31.488 | 1.000 | 34.93 |
| ATOM | 249 | CA  | GLU | A | 49 | 11.443 | 21.484 | 31.313 | 1.000 | 36.05 |
| ATOM | 250 | CB  | GLU | A | 49 | 11.210 | 22.881 | 31.875 | 1.000 | 45.26 |
| ATOM | 251 | CG  | GLU | A | 49 | 11.239 | 22.953 | 33.390 | 1.000 | 56.89 |
| ATOM | 252 | CD  | GLU | A | 49 | 10.271 | 21.998 | 34.053 | 1.000 | 65.15 |
| ATOM | 253 | OE1 | GLU | A | 49 | 10.722 | 21.031 | 34.704 | 1.000 | 61.85 |
| ATOM | 254 | OE2 | GLU | A | 49 | 9.047  | 22.220 | 33.926 | 1.000 | 85.66 |
| ATOM | 255 | C   | GLU | A | 49 | 11.065 | 21.406 | 29.835 | 1.000 | 40.11 |
| ATOM | 256 | O   | GLU | A | 49 | 9.884  | 21.429 | 29.488 | 1.000 | 45.25 |
| ATOM | 257 | N   | GLU | A | 50 | 12.071 | 21.304 | 28.972 | 1.000 | 34.88 |
| ATOM | 258 | CA  | GLU | A | 50 | 11.897 | 21.219 | 27.536 | 1.000 | 34.15 |
| ATOM | 259 | CB  | GLU | A | 50 | 13.225 | 21.224 | 26.784 | 1.000 | 47.42 |

**FIGURE 11**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 260 | CG  | GLU | A | 50 | 14.193 | 22.357 | 27.039 | 1.000 | 58.31 |
| ATOM | 261 | CD  | GLU | A | 50 | 15.395 | 22.299 | 26.111 | 1.000 | 72.71 |
| ATOM | 262 | OE1 | GLU | A | 50 | 15.705 | 21.201 | 25.592 | 1.000 | 84.88 |
| ATOM | 263 | OE2 | GLU | A | 50 | 16.034 | 23.355 | 25.892 | 1.000 | 89.36 |
| ATOM | 264 | C   | GLU | A | 50 | 11.172 | 19.927 | 27.145 | 1.000 | 41.10 |
| ATOM | 265 | O   | GLU | A | 50 | 10.637 | 19.814 | 26.042 | 1.000 | 48.55 |
| ATOM | 266 | N   | LEU | A | 51 | 11.214 | 18.984 | 28.077 | 1.000 | 37.69 |
| ATOM | 267 | CA  | LEU | A | 51 | 10.671 | 17.650 | 27.907 | 1.000 | 34.93 |
| ATOM | 268 | CB  | LEU | A | 51 | 11.632 | 16.647 | 28.554 | 1.000 | 32.69 |
| ATOM | 269 | CG  | LEU | A | 51 | 12.990 | 16.479 | 27.869 | 1.000 | 27.26 |
| ATOM | 270 | CD1 | LEU | A | 51 | 14.003 | 15.896 | 28.837 | 1.000 | 30.09 |
| ATOM | 271 | CD2 | LEU | A | 51 | 12.860 | 15.598 | 26.636 | 1.000 | 25.80 |
| ATOM | 272 | C   | LEU | A | 51 | 9.286  | 17.512 | 28.523 | 1.000 | 39.93 |
| ATOM | 273 | O   | LEU | A | 51 | 8.633  | 16.483 | 28.348 | 1.000 | 32.60 |
| ATOM | 274 | N   | LYS | A | 52 | 8.856  | 18.542 | 29.242 | 1.000 | 35.85 |
| ATOM | 275 | CA  | LYS | A | 52 | 7.628  | 18.496 | 30.017 | 1.000 | 43.68 |
| ATOM | 276 | CB  | LYS | A | 52 | 7.282  | 19.881 | 30.584 | 1.000 | 49.99 |
| ATOM | 277 | CG  | LYS | A | 52 | 5.828  | 20.014 | 31.009 | 1.000 | 50.93 |
| ATOM | 278 | CD  | LYS | A | 52 | 5.552  | 21.383 | 31.613 | 1.000 | 54.40 |
| ATOM | 279 | CE  | LYS | A | 52 | 4.187  | 21.908 | 31.183 | 1.000 | 52.01 |
| ATOM | 280 | NZ  | LYS | A | 52 | 4.061  | 23.372 | 31.421 | 1.000 | 52.88 |
| ATOM | 281 | C   | LYS | A | 52 | 6.440  | 17.978 | 29.211 | 1.000 | 41.72 |
| ATOM | 282 | O   | LYS | A | 52 | 5.749  | 17.087 | 29.712 | 1.000 | 40.74 |
| ATOM | 283 | N   | ASP | A | 53 | 6.241  | 18.521 | 28.018 | 1.000 | 35.76 |
| ATOM | 284 | CA  | ASP | A | 53 | 5.074  | 18.259 | 27.196 | 1.000 | 33.00 |
| ATOM | 285 | CB  | ASP | A | 53 | 4.640  | 19.524 | 26.440 | 1.000 | 35.62 |
| ATOM | 286 | CG  | ASP | A | 53 | 4.134  | 20.637 | 27.333 | 1.000 | 39.83 |
| ATOM | 287 | OD1 | ASP | A | 53 | 4.039  | 21.790 | 26.856 | 1.000 | 41.69 |
| ATOM | 288 | OD2 | ASP | A | 53 | 3.834  | 20.393 | 28.518 | 1.000 | 48.93 |
| ATOM | 289 | C   | ASP | A | 53 | 5.283  | 17.142 | 26.177 | 1.000 | 29.06 |
| ATOM | 290 | O   | ASP | A | 53 | 4.349  | 16.827 | 25.426 | 1.000 | 22.95 |
| ATOM | 291 | N   | VAL | A | 54 | 6.459  | 16.533 | 26.120 | 1.000 | 26.91 |
| ATOM | 292 | CA  | VAL | A | 54 | 6.661  | 15.454 | 25.148 | 1.000 | 23.54 |
| ATOM | 293 | CB  | VAL | A | 54 | 8.059  | 14.818 | 25.272 | 1.000 | 30.36 |
| ATOM | 294 | CG1 | VAL | A | 54 | 8.120  | 13.547 | 24.435 | 1.000 | 21.06 |
| ATOM | 295 | CG2 | VAL | A | 54 | 9.154  | 15.791 | 24.855 | 1.000 | 31.51 |
| ATOM | 296 | C   | VAL | A | 54 | 5.617  | 14.348 | 25.309 | 1.000 | 29.36 |
| ATOM | 297 | O   | VAL | A | 54 | 5.350  | 13.848 | 26.409 | 1.000 | 28.89 |
| ATOM | 298 | N   | GLY | A | 55 | 5.015  | 13.988 | 24.188 | 1.000 | 23.19 |
| ATOM | 299 | CA  | GLY | A | 55 | 4.021  | 12.953 | 24.067 | 1.000 | 23.74 |
| ATOM | 300 | C   | GLY | A | 55 | 2.731  | 13.216 | 24.816 | 1.000 | 35.64 |
| ATOM | 301 | O   | GLY | A | 55 | 1.917  | 12.289 | 24.916 | 1.000 | 34.29 |
| ATOM | 302 | N   | ARG | A | 56 | 2.535  | 14.432 | 25.331 | 1.000 | 26.60 |
| ATOM | 303 | CA  | ARG | A | 56 | 1.351  | 14.736 | 26.122 | 1.000 | 26.13 |
| ATOM | 304 | CB  | ARG | A | 56 | 1.587  | 15.960 | 27.020 | 1.000 | 28.53 |
| ATOM | 305 | CG  | ARG | A | 56 | 2.477  | 15.672 | 28.222 | 1.000 | 31.24 |
| ATOM | 306 | CD  | ARG | A | 56 | 1.970  | 14.486 | 29.030 | 1.000 | 31.18 |
| ATOM | 307 | NE  | ARG | A | 56 | 2.866  | 14.160 | 30.136 | 1.000 | 39.70 |
| ATOM | 308 | CZ  | ARG | A | 56 | 2.724  | 14.463 | 31.417 | 1.000 | 41.60 |
| ATOM | 309 | NH1 | ARG | A | 56 | 1.683  | 15.139 | 31.879 | 1.000 | 33.99 |
| ATOM | 310 | NH2 | ARG | A | 56 | 3.650  | 14.082 | 32.292 | 1.000 | 42.42 |
| ATOM | 311 | C   | ARG | A | 56 | 0.123  | 14.966 | 25.250 | 1.000 | 24.97 |

**FIGURE 12**



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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 312 | O   | ARG | A | 56 | -0.957  | 15.301 | 25.741 | 1.000 | 29.55 |
| ATOM | 313 | N   | ASN | A | 57 | 0.258   | 14.781 | 23.944 | 1.000 | 24.28 |
| ATOM | 314 | CA  | ASN | A | 57 | -0.895  | 14.909 | 23.064 | 1.000 | 33.49 |
| ATOM | 315 | CB  | ASN | A | 57 | -0.474  | 15.189 | 21.611 | 1.000 | 33.93 |
| ATOM | 316 | CG  | ASN | A | 57 | 0.605   | 14.218 | 21.162 | 1.000 | 35.19 |
| ATOM | 317 | OD1 | ASN | A | 57 | 1.492   | 13.907 | 21.957 | 1.000 | 42.76 |
| ATOM | 318 | ND2 | ASN | A | 57 | 0.547   | 13.751 | 19.918 | 1.000 | 35.98 |
| ATOM | 319 | C   | ASN | A | 57 | -1.720  | 13.635 | 23.056 | 1.000 | 35.77 |
| ATOM | 320 | O   | ASN | A | 57 | -2.865  | 13.607 | 22.617 | 1.000 | 32.52 |
| ATOM | 321 | N   | GLN | A | 58 | -1.139  | 12.529 | 23.521 | 1.000 | 35.76 |
| ATOM | 322 | CA  | GLN | A | 58 | -1.864  | 11.271 | 23.295 | 1.000 | 30.59 |
| ATOM | 323 | CB  | GLN | A | 58 | -0.851  | 10.129 | 23.178 | 1.000 | 29.64 |
| ATOM | 324 | CG  | GLN | A | 58 | 0.201   | 10.442 | 22.108 | 1.000 | 28.67 |
| ATOM | 325 | CD  | GLN | A | 58 | 1.406   | 9.527  | 22.230 | 1.000 | 31.92 |
| ATOM | 326 | OE1 | GLN | A | 58 | 2.330   | 9.754  | 23.023 | 1.000 | 40.11 |
| ATOM | 327 | NE2 | GLN | A | 58 | 1.386   | 8.474  | 21.427 | 1.000 | 22.80 |
| ATOM | 328 | C   | GLN | A | 58 | -2.899  | 11.017 | 24.373 | 1.000 | 26.57 |
| ATOM | 329 | O   | GLN | A | 58 | -2.814  | 11.505 | 25.494 | 1.000 | 28.16 |
| ATOM | 330 | N   | SER | A | 59 | -3.895  | 10.232 | 23.996 | 1.000 | 21.64 |
| ATOM | 331 | CA  | SER | A | 59 | -5.004  | 9.889  | 24.858 | 1.000 | 21.49 |
| ATOM | 332 | CB  | SER | A | 59 | -6.312  | 9.936  | 24.060 | 1.000 | 23.13 |
| ATOM | 333 | OG  | SER | A | 59 | -6.423  | 8.760  | 23.266 | 1.000 | 50.75 |
| ATOM | 334 | C   | SER | A | 59 | -4.832  | 8.495  | 25.465 | 1.000 | 27.34 |
| ATOM | 335 | O   | SER | A | 59 | -4.113  | 7.652  | 24.915 | 1.000 | 28.20 |
| ATOM | 336 | N   | CYS | A | 60 | -5.510  | 8.289  | 26.585 | 1.000 | 21.68 |
| ATOM | 337 | CA  | CYS | A | 60 | -5.566  | 7.030  | 27.307 | 1.000 | 19.90 |
| ATOM | 338 | CB  | CYS | A | 60 | -4.841  | 7.171  | 28.645 | 1.000 | 31.73 |
| ATOM | 339 | SG  | CYS | A | 60 | -3.240  | 8.002  | 28.554 | 1.000 | 43.81 |
| ATOM | 340 | C   | CYS | A | 60 | -7.008  | 6.595  | 27.556 | 1.000 | 22.77 |
| ATOM | 341 | O   | CYS | A | 60 | -7.341  | 6.204  | 28.678 | 1.000 | 20.42 |
| ATOM | 342 | N   | ASP | A | 61 | -7.852  | 6.663  | 26.540 | 1.000 | 21.77 |
| ATOM | 343 | CA  | ASP | A | 61 | -9.266  | 6.323  | 26.610 | 1.000 | 30.03 |
| ATOM | 344 | CB  | ASP | A | 61 | -9.915  | 6.527  | 25.236 | 1.000 | 35.37 |
| ATOM | 345 | CG  | ASP | A | 61 | -9.894  | 7.936  | 24.695 | 1.000 | 32.99 |
| ATOM | 346 | OD1 | ASP | A | 61 | -9.618  | 8.909  | 25.426 | 1.000 | 42.37 |
| ATOM | 347 | OD2 | ASP | A | 61 | -10.171 | 8.083  | 23.481 | 1.000 | 42.70 |
| ATOM | 348 | C   | ASP | A | 61 | -9.529  | 4.890  | 27.073 | 1.000 | 31.27 |
| ATOM | 349 | O   | ASP | A | 61 | -10.375 | 4.669  | 27.946 | 1.000 | 26.07 |
| ATOM | 350 | N   | ILE | A | 62 | -8.840  | 3.896  | 26.517 | 1.000 | 33.57 |
| ATOM | 351 | CA  | ILE | A | 62 | -9.017  | 2.497  | 26.889 | 1.000 | 26.85 |
| ATOM | 352 | CB  | ILE | A | 62 | -8.021  | 1.572  | 26.166 | 1.000 | 27.84 |
| ATOM | 353 | CG1 | ILE | A | 62 | -7.987  | 1.728  | 24.650 | 1.000 | 25.02 |
| ATOM | 354 | CD1 | ILE | A | 62 | -9.326  | 1.502  | 23.982 | 1.000 | 31.68 |
| ATOM | 355 | CG2 | ILE | A | 62 | -8.284  | 0.124  | 26.574 | 1.000 | 22.54 |
| ATOM | 356 | C   | ILE | A | 62 | -8.822  | 2.256  | 28.381 | 1.000 | 32.08 |
| ATOM | 357 | O   | ILE | A | 62 | -9.608  | 1.599  | 29.071 | 1.000 | 30.72 |
| ATOM | 358 | N   | ALA | A | 63 | -7.724  | 2.812  | 28.896 | 1.000 | 25.21 |
| ATOM | 359 | CA  | ALA | A | 63 | -7.448  | 2.650  | 30.321 | 1.000 | 24.51 |
| ATOM | 360 | CB  | ALA | A | 63 | -6.138  | 3.336  | 30.687 | 1.000 | 24.25 |
| ATOM | 361 | C   | ALA | A | 63 | -8.585  | 3.208  | 31.168 | 1.000 | 32.19 |
| ATOM | 362 | O   | ALA | A | 63 | -8.795  | 2.776  | 32.302 | 1.000 | 36.44 |
| ATOM | 363 | N   | LEU | A | 64 | -9.309  | 4.183  | 30.622 | 1.000 | 29.54 |

**FIGURE 13**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 364 | CA  | LEU | A | 64 | -10.325 | 4.890  | 31.389 | 1.000 | 31.43 |
| ATOM | 365 | CB  | LEU | A | 64 | -10.486 | 6.331  | 30.884 | 1.000 | 27.77 |
| ATOM | 366 | CG  | LEU | A | 64 | -9.333  | 7.259  | 31.283 | 1.000 | 27.38 |
| ATOM | 367 | CD1 | LEU | A | 64 | -9.308  | 8.494  | 30.399 | 1.000 | 15.84 |
| ATOM | 368 | CD2 | LEU | A | 64 | -9.456  | 7.608  | 32.760 | 1.000 | 25.15 |
| ATOM | 369 | C   | LEU | A | 64 | -11.663 | 4.180  | 31.315 | 1.000 | 27.53 |
| ATOM | 370 | O   | LEU | A | 64 | -12.640 | 4.639  | 31.902 | 1.000 | 25.88 |
| ATOM | 371 | N   | LEU | A | 65 | -11.712 | 3.063  | 30.594 | 1.000 | 24.50 |
| ATOM | 372 | CA  | LEU | A | 65 | -13.005 | 2.371  | 30.555 | 1.000 | 29.09 |
| ATOM | 373 | CB  | LEU | A | 65 | -12.934 | 1.238  | 29.534 | 1.000 | 26.20 |
| ATOM | 374 | CG  | LEU | A | 65 | -12.633 | 1.726  | 28.112 | 1.000 | 32.04 |
| ATOM | 375 | CD1 | LEU | A | 65 | -12.556 | 0.568  | 27.137 | 1.000 | 26.24 |
| ATOM | 376 | CD2 | LEU | A | 65 | -13.692 | 2.740  | 27.692 | 1.000 | 42.91 |
| ATOM | 377 | C   | LEU | A | 65 | -13.380 | 1.876  | 31.948 | 1.000 | 36.19 |
| ATOM | 378 | O   | LEU | A | 65 | -12.506 | 1.424  | 32.690 | 1.000 | 34.08 |
| ATOM | 379 | N   | PRO | A | 66 | -14.658 | 1.985  | 32.302 | 1.000 | 38.51 |
| ATOM | 380 | CA  | PRO | A | 66 | -15.156 | 1.575  | 33.618 | 1.000 | 45.55 |
| ATOM | 381 | CB  | PRO | A | 66 | -16.682 | 1.595  | 33.438 | 1.000 | 41.37 |
| ATOM | 382 | CG  | PRO | A | 66 | -16.895 | 2.654  | 32.411 | 1.000 | 38.85 |
| ATOM | 383 | CD  | PRO | A | 66 | -15.733 | 2.545  | 31.463 | 1.000 | 39.79 |
| ATOM | 384 | C   | PRO | A | 66 | -14.718 | 0.173  | 34.026 | 1.000 | 45.91 |
| ATOM | 385 | O   | PRO | A | 66 | -14.329 | -0.049 | 35.171 | 1.000 | 40.19 |
| ATOM | 386 | N   | GLU | A | 67 | -14.780 | -0.764 | 33.090 | 1.000 | 39.45 |
| ATOM | 387 | CA  | GLU | A | 67 | -14.412 | -2.143 | 33.370 | 1.000 | 36.99 |
| ATOM | 388 | CB  | GLU | A | 67 | -14.780 | -3.022 | 32.170 | 1.000 | 40.26 |
| ATOM | 389 | CG  | GLU | A | 67 | -13.872 | -2.765 | 30.975 | 1.000 | 51.03 |
| ATOM | 390 | CD  | GLU | A | 67 | -14.478 | -3.329 | 29.706 | 1.000 | 62.19 |
| ATOM | 391 | OE1 | GLU | A | 67 | -15.190 | -4.351 | 29.789 | 1.000 | 95.02 |
| ATOM | 392 | OE2 | GLU | A | 67 | -14.229 | -2.750 | 28.629 | 1.000 | 48.12 |
| ATOM | 393 | C   | GLU | A | 67 | -12.929 | -2.311 | 33.685 | 1.000 | 41.35 |
| ATOM | 394 | O   | GLU | A | 67 | -12.555 | -3.306 | 34.309 | 1.000 | 49.39 |
| ATOM | 395 | N   | ASN | A | 68 | -12.105 | -1.357 | 33.266 | 1.000 | 44.36 |
| ATOM | 396 | CA  | ASN | A | 68 | -10.668 | -1.381 | 33.488 | 1.000 | 35.22 |
| ATOM | 397 | CB  | ASN | A | 68 | -9.938  | -0.853 | 32.244 | 1.000 | 30.80 |
| ATOM | 398 | CG  | ASN | A | 68 | -10.071 | -1.799 | 31.070 | 1.000 | 26.82 |
| ATOM | 399 | OD1 | ASN | A | 68 | -10.219 | -3.004 | 31.263 | 1.000 | 30.94 |
| ATOM | 400 | ND2 | ASN | A | 68 | -10.021 | -1.271 | 29.849 | 1.000 | 25.55 |
| ATOM | 401 | C   | ASN | A | 68 | -10.240 | -0.570 | 34.706 | 1.000 | 35.99 |
| ATOM | 402 | O   | ASN | A | 68 | -9.074  | -0.612 | 35.110 | 1.000 | 34.21 |
| ATOM | 403 | N   | ARG | A | 69 | -11.151 | 0.170  | 35.325 | 1.000 | 40.53 |
| ATOM | 404 | CA  | ARG | A | 69 | -10.796 | 1.005  | 36.475 | 1.000 | 35.31 |
| ATOM | 405 | CB  | ARG | A | 69 | -12.060 | 1.688  | 36.993 | 1.000 | 47.65 |
| ATOM | 406 | CG  | ARG | A | 69 | -11.878 | 3.089  | 37.547 | 1.000 | 59.36 |
| ATOM | 407 | CD  | ARG | A | 69 | -12.710 | 3.262  | 38.819 | 1.000 | 65.36 |
| ATOM | 408 | NE  | ARG | A | 69 | -12.615 | 2.076  | 39.666 | 1.000 | 69.47 |
| ATOM | 409 | CZ  | ARG | A | 69 | -13.019 | 1.980  | 40.923 | 1.000 | 75.71 |
| ATOM | 410 | NH1 | ARG | A | 69 | -13.586 | 3.018  | 41.542 | 1.000 | 91.00 |
| ATOM | 411 | NH2 | ARG | A | 69 | -12.880 | 0.832  | 41.575 | 1.000 | 74.09 |
| ATOM | 412 | C   | ARG | A | 69 | -10.114 | 0.205  | 37.572 | 1.000 | 33.70 |
| ATOM | 413 | O   | ARG | A | 69 | -9.102  | 0.634  | 38.135 | 1.000 | 41.23 |
| ATOM | 414 | N   | GLY | A | 70 | -10.641 | -0.976 | 37.890 | 1.000 | 34.09 |
| ATOM | 415 | CA  | GLY | A | 70 | -10.030 | -1.844 | 38.877 | 1.000 | 29.32 |

**FIGURE 14**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 416 | C   | GLY | A | 70 | -8.645  | -2.304 | 38.476 | 1.000 | 33.87 |
| ATOM | 417 | O   | GLY | A | 70 | -7.861  | -2.788 | 39.293 | 1.000 | 29.15 |
| ATOM | 418 | N   | LYS | A | 71 | -8.269  | -2.166 | 37.200 | 1.000 | 28.62 |
| ATOM | 419 | CA  | LYS | A | 71 | -6.975  | -2.730 | 36.805 | 1.000 | 28.56 |
| ATOM | 420 | CB  | LYS | A | 71 | -7.145  | -3.327 | 35.403 | 1.000 | 26.54 |
| ATOM | 421 | CG  | LYS | A | 71 | -8.206  | -4.431 | 35.340 | 1.000 | 22.84 |
| ATOM | 422 | CD  | LYS | A | 71 | -8.540  | -4.715 | 33.880 | 1.000 | 25.18 |
| ATOM | 423 | CE  | LYS | A | 71 | -9.766  | -5.603 | 33.744 | 1.000 | 26.92 |
| ATOM | 424 | NZ  | LYS | A | 71 | -10.179 | -5.703 | 32.310 | 1.000 | 25.36 |
| ATOM | 425 | C   | LYS | A | 71 | -5.825  | -1.737 | 36.871 | 1.000 | 24.24 |
| ATOM | 426 | O   | LYS | A | 71 | -4.670  | -2.046 | 36.565 | 1.000 | 23.92 |
| ATOM | 427 | N   | ASN | A | 72 | -6.078  | -0.506 | 37.292 | 1.000 | 21.36 |
| ATOM | 428 | CA  | ASN | A | 72 | -5.019  | 0.485  | 37.438 | 1.000 | 22.33 |
| ATOM | 429 | CB  | ASN | A | 72 | -5.431  | 1.802  | 36.760 | 1.000 | 17.72 |
| ATOM | 430 | CG  | ASN | A | 72 | -5.773  | 1.557  | 35.299 | 1.000 | 20.67 |
| ATOM | 431 | OD1 | ASN | A | 72 | -4.968  | 1.023  | 34.534 | 1.000 | 19.13 |
| ATOM | 432 | ND2 | ASN | A | 72 | -6.981  | 1.935  | 34.901 | 1.000 | 22.56 |
| ATOM | 433 | C   | ASN | A | 72 | -4.691  | 0.708  | 38.904 | 1.000 | 22.55 |
| ATOM | 434 | O   | ASN | A | 72 | -5.548  | 0.952  | 39.747 | 1.000 | 27.49 |
| ATOM | 435 | N   | ARG | A | 73 | -3.410  | 0.626  | 39.238 | 1.000 | 24.79 |
| ATOM | 436 | CA  | ARG | A | 73 | -2.989  | 0.857  | 40.612 | 1.000 | 22.71 |
| ATOM | 437 | CB  | ARG | A | 73 | -1.523  | 0.471  | 40.761 | 1.000 | 19.16 |
| ATOM | 438 | CG  | ARG | A | 73 | -1.003  | 0.559  | 42.185 | 1.000 | 20.59 |
| ATOM | 439 | CD  | ARG | A | 73 | 0.456   | 0.114  | 42.254 | 1.000 | 16.95 |
| ATOM | 440 | NE  | ARG | A | 73 | 0.546   | -1.347 | 42.281 | 1.000 | 17.30 |
| ATOM | 441 | CZ  | ARG | A | 73 | 0.282   | -2.041 | 43.387 | 1.000 | 28.69 |
| ATOM | 442 | NH1 | ARG | A | 73 | -0.073  | -1.406 | 44.500 | 1.000 | 20.46 |
| ATOM | 443 | NH2 | ARG | A | 73 | 0.372   | -3.371 | 43.383 | 1.000 | 26.38 |
| ATOM | 444 | C   | ARG | A | 73 | -3.227  | 2.314  | 40.990 | 1.000 | 29.57 |
| ATOM | 445 | O   | ARG | A | 73 | -3.731  | 2.609  | 42.070 | 1.000 | 23.74 |
| ATOM | 446 | N   | TYR | A | 74 | -2.864  | 3.229  | 40.095 | 1.000 | 22.89 |
| ATOM | 447 | CA  | TYR | A | 74 | -3.188  | 4.640  | 40.292 | 1.000 | 19.10 |
| ATOM | 448 | CB  | TYR | A | 74 | -1.941  | 5.487  | 40.496 | 1.000 | 29.90 |
| ATOM | 449 | CG  | TYR | A | 74 | -0.889  | 4.936  | 41.434 | 1.000 | 28.85 |
| ATOM | 450 | CD1 | TYR | A | 74 | -0.948  | 5.169  | 42.802 | 1.000 | 29.68 |
| ATOM | 451 | CE1 | TYR | A | 74 | 0.019   | 4.668  | 43.655 | 1.000 | 32.91 |
| ATOM | 452 | CZ  | TYR | A | 74 | 1.064   | 3.920  | 43.146 | 1.000 | 32.73 |
| ATOM | 453 | OH  | TYR | A | 74 | 2.029   | 3.415  | 43.989 | 1.000 | 28.80 |
| ATOM | 454 | CE2 | TYR | A | 74 | 1.156   | 3.672  | 41.791 | 1.000 | 20.37 |
| ATOM | 455 | CD2 | TYR | A | 74 | 0.182   | 4.186  | 40.957 | 1.000 | 22.57 |
| ATOM | 456 | C   | TYR | A | 74 | -4.007  | 5.110  | 39.095 | 1.000 | 33.71 |
| ATOM | 457 | O   | TYR | A | 74 | -3.753  | 4.819  | 37.920 | 1.000 | 23.30 |
| ATOM | 458 | N   | ASN | A | 75 | -5.062  | 5.861  | 39.410 | 1.000 | 33.95 |
| ATOM | 459 | CA  | ASN | A | 75 | -6.019  | 6.213  | 38.358 | 1.000 | 32.58 |
| ATOM | 460 | CB  | ASN | A | 75 | -7.389  | 6.458  | 39.014 | 1.000 | 35.23 |
| ATOM | 461 | CG  | ASN | A | 75 | -7.716  | 5.300  | 39.947 | 1.000 | 42.60 |
| ATOM | 462 | OD1 | ASN | A | 75 | -7.925  | 5.491  | 41.144 | 1.000 | 68.26 |
| ATOM | 463 | ND2 | ASN | A | 75 | -7.745  | 4.087  | 39.403 | 1.000 | 39.56 |
| ATOM | 464 | C   | ASN | A | 75 | -5.533  | 7.385  | 37.534 | 1.000 | 30.63 |
| ATOM | 465 | O   | ASN | A | 75 | -6.101  | 7.736  | 36.497 | 1.000 | 26.15 |
| ATOM | 466 | N   | ASN | A | 76 | -4.440  | 8.015  | 37.962 | 1.000 | 28.76 |
| ATOM | 467 | CA  | ASN | A | 76 | -3.897  | 9.102  | 37.150 | 1.000 | 28.13 |

**FIGURE 15**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 468 | CB  | ASN | A | 76 | -3.719 | 10.374 | 37.979 | 1.000 | 27.74 |
| ATOM | 469 | CG  | ASN | A | 76 | -2.648 | 10.200 | 39.041 | 1.000 | 28.93 |
| ATOM | 470 | OD1 | ASN | A | 76 | -2.497 | 9.101  | 39.573 | 1.000 | 29.34 |
| ATOM | 471 | ND2 | ASN | A | 76 | -1.937 | 11.284 | 39.321 | 1.000 | 29.63 |
| ATOM | 472 | C   | ASN | A | 76 | -2.570 | 8.694  | 36.526 | 1.000 | 29.10 |
| ATOM | 473 | O   | ASN | A | 76 | -1.851 | 9.557  | 36.015 | 1.000 | 33.33 |
| ATOM | 474 | N   | ILE | A | 77 | -2.273 | 7.392  | 36.558 | 1.000 | 24.17 |
| ATOM | 475 | CA  | ILE | A | 77 | -1.095 | 6.908  | 35.830 | 1.000 | 23.94 |
| ATOM | 476 | CB  | ILE | A | 77 | 0.024  | 6.496  | 36.797 | 1.000 | 28.53 |
| ATOM | 477 | CG1 | ILE | A | 77 | 0.575  | 7.663  | 37.624 | 1.000 | 24.03 |
| ATOM | 478 | CD1 | ILE | A | 77 | 1.451  | 7.212  | 38.776 | 1.000 | 35.26 |
| ATOM | 479 | CG2 | ILE | A | 77 | 1.137  | 5.798  | 36.041 | 1.000 | 21.08 |
| ATOM | 480 | C   | ILE | A | 77 | -1.457 | 5.760  | 34.900 | 1.000 | 22.75 |
| ATOM | 481 | O   | ILE | A | 77 | -1.618 | 4.597  | 35.282 | 1.000 | 17.56 |
| ATOM | 482 | N   | LEU | A | 78 | -1.605 | 6.108  | 33.621 | 1.000 | 16.56 |
| ATOM | 483 | CA  | LEU | A | 78 | -2.172 | 5.202  | 32.641 | 1.000 | 12.89 |
| ATOM | 484 | CB  | LEU | A | 78 | -3.616 | 5.616  | 32.310 | 1.000 | 17.17 |
| ATOM | 485 | CG  | LEU | A | 78 | -4.457 | 6.017  | 33.522 | 1.000 | 22.43 |
| ATOM | 486 | CD1 | LEU | A | 78 | -5.794 | 6.590  | 33.075 | 1.000 | 27.35 |
| ATOM | 487 | CD2 | LEU | A | 78 | -4.637 | 4.813  | 34.431 | 1.000 | 17.32 |
| ATOM | 488 | C   | LEU | A | 78 | -1.415 | 5.213  | 31.326 | 1.000 | 17.93 |
| ATOM | 489 | O   | LEU | A | 78 | -0.846 | 6.221  | 30.922 | 1.000 | 18.95 |
| ATOM | 490 | N   | PRO | A | 79 | -1.459 | 4.086  | 30.640 | 1.000 | 21.12 |
| ATOM | 491 | CA  | PRO | A | 79 | -0.773 | 3.971  | 29.355 | 1.000 | 18.86 |
| ATOM | 492 | CB  | PRO | A | 79 | -0.858 | 2.470  | 29.068 | 1.000 | 18.12 |
| ATOM | 493 | CG  | PRO | A | 79 | -2.148 | 2.076  | 29.721 | 1.000 | 21.28 |
| ATOM | 494 | CD  | PRO | A | 79 | -2.184 | 2.858  | 31.011 | 1.000 | 17.43 |
| ATOM | 495 | C   | PRO | A | 79 | -1.532 | 4.694  | 28.253 | 1.000 | 19.81 |
| ATOM | 496 | O   | PRO | A | 79 | -2.761 | 4.633  | 28.249 | 1.000 | 19.07 |
| ATOM | 497 | N   | TYR | A | 80 | -0.784 | 5.317  | 27.355 | 1.000 | 16.14 |
| ATOM | 498 | CA  | TYR | A | 80 | -1.338 | 5.843  | 26.117 | 1.000 | 15.09 |
| ATOM | 499 | CB  | TYR | A | 80 | -0.216 | 6.508  | 25.313 | 1.000 | 20.99 |
| ATOM | 500 | CG  | TYR | A | 80 | 0.350  | 7.734  | 25.993 | 1.000 | 20.29 |
| ATOM | 501 | CD1 | TYR | A | 80 | -0.494 | 8.670  | 26.577 | 1.000 | 20.64 |
| ATOM | 502 | CE1 | TYR | A | 80 | 0.019  | 9.796  | 27.206 | 1.000 | 20.96 |
| ATOM | 503 | CZ  | TYR | A | 80 | 1.385  | 9.986  | 27.243 | 1.000 | 21.66 |
| ATOM | 504 | OH  | TYR | A | 80 | 1.903  | 11.103 | 27.859 | 1.000 | 23.51 |
| ATOM | 505 | CE2 | TYR | A | 80 | 2.239  | 9.071  | 26.671 | 1.000 | 18.25 |
| ATOM | 506 | CD2 | TYR | A | 80 | 1.722  | 7.946  | 26.047 | 1.000 | 21.75 |
| ATOM | 507 | C   | TYR | A | 80 | -1.988 | 4.755  | 25.277 | 1.000 | 23.46 |
| ATOM | 508 | O   | TYR | A | 80 | -1.471 | 3.635  | 25.187 | 1.000 | 23.99 |
| ATOM | 509 | N   | ASP | A | 81 | -3.125 | 5.040  | 24.637 | 1.000 | 22.91 |
| ATOM | 510 | CA  | ASP | A | 81 | -3.735 | 4.027  | 23.780 | 1.000 | 19.34 |
| ATOM | 511 | CB  | ASP | A | 81 | -5.033 | 4.518  | 23.120 | 1.000 | 24.22 |
| ATOM | 512 | CG  | ASP | A | 81 | -6.080 | 4.908  | 24.143 | 1.000 | 34.31 |
| ATOM | 513 | OD1 | ASP | A | 81 | -6.296 | 4.128  | 25.094 | 1.000 | 27.78 |
| ATOM | 514 | OD2 | ASP | A | 81 | -6.688 | 5.992  | 24.010 | 1.000 | 35.52 |
| ATOM | 515 | C   | ASP | A | 81 | -2.769 | 3.610  | 22.678 | 1.000 | 18.44 |
| ATOM | 516 | O   | ASP | A | 81 | -2.722 | 2.439  | 22.278 | 1.000 | 24.18 |
| ATOM | 517 | N   | ALA | A | 82 | -2.002 | 4.573  | 22.161 | 1.000 | 16.71 |
| ATOM | 518 | CA  | ALA | A | 82 | -1.164 | 4.229  | 21.008 | 1.000 | 21.74 |
| ATOM | 519 | CB  | ALA | A | 82 | -0.654 | 5.520  | 20.373 | 1.000 | 25.83 |

**FIGURE 16**

|      |     |     |     |   |    |        |         |        |       |       |
|------|-----|-----|-----|---|----|--------|---------|--------|-------|-------|
| ATOM | 520 | C   | ALA | A | 82 | -0.010 | 3.300   | 21.338 | 1.000 | 26.28 |
| ATOM | 521 | O   | ALA | A | 82 | 0.556  | 2.660   | 20.439 | 1.000 | 24.04 |
| ATOM | 522 | N   | THR | A | 83 | 0.447  | 3.140   | 22.584 | 1.000 | 19.03 |
| ATOM | 523 | CA  | THR | A | 83 | 1.625  | 2.280   | 22.757 | 1.000 | 14.68 |
| ATOM | 524 | CB  | THR | A | 83 | 2.853  | 3.095   | 23.225 | 1.000 | 22.79 |
| ATOM | 525 | OG1 | THR | A | 83 | 2.464  | 3.852   | 24.374 | 1.000 | 18.61 |
| ATOM | 526 | CG2 | THR | A | 83 | 3.308  | 4.096   | 22.168 | 1.000 | 17.97 |
| ATOM | 527 | C   | THR | A | 83 | 1.412  | 1.199   | 23.799 | 1.000 | 22.48 |
| ATOM | 528 | O   | THR | A | 83 | 2.380  | 0.580   | 24.254 | 1.000 | 20.29 |
| ATOM | 529 | N   | ARG | A | 84 | 0.144  | 1.005   | 24.159 | 1.000 | 18.73 |
| ATOM | 530 | CA  | ARG | A | 84 | -0.176 | 0.106   | 25.257 | 1.000 | 22.92 |
| ATOM | 531 | CB  | ARG | A | 84 | -1.621 | 0.347   | 25.683 | 1.000 | 27.10 |
| ATOM | 532 | CG  | ARG | A | 84 | -2.650 | -0.247  | 24.721 | 1.000 | 21.68 |
| ATOM | 533 | CD  | ARG | A | 84 | -4.047 | 0.092   | 25.236 | 1.000 | 25.76 |
| ATOM | 534 | NE  | ARG | A | 84 | -5.071 | -0.515  | 24.395 | 1.000 | 31.14 |
| ATOM | 535 | CZ  | ARG | A | 84 | -5.698 | -1.652  | 24.648 | 1.000 | 28.06 |
| ATOM | 536 | NH1 | ARG | A | 84 | -5.426 | -2.351  | 25.741 | 1.000 | 15.53 |
| ATOM | 537 | NH2 | ARG | A | 84 | -6.608 | -2.073  | 23.781 | 1.000 | 24.30 |
| ATOM | 538 | C   | ARG | A | 84 | 0.032  | -1.353  | 24.874 | 1.000 | 25.02 |
| ATOM | 539 | O   | ARG | A | 84 | -0.089 | -1.712  | 23.702 | 1.000 | 21.04 |
| ATOM | 540 | N   | VAL | A | 85 | 0.337  | -2.204  | 25.856 | 1.000 | 14.13 |
| ATOM | 541 | CA  | VAL | A | 85 | 0.491  | -3.624  | 25.512 | 1.000 | 14.38 |
| ATOM | 542 | CB  | VAL | A | 85 | 1.464  | -4.344  | 26.455 | 1.000 | 9.78  |
| ATOM | 543 | CG1 | VAL | A | 85 | 1.425  | -5.848  | 26.218 | 1.000 | 17.73 |
| ATOM | 544 | CG2 | VAL | A | 85 | 2.881  | -3.814  | 26.306 | 1.000 | 12.51 |
| ATOM | 545 | C   | VAL | A | 85 | -0.863 | -4.313  | 25.593 | 1.000 | 24.23 |
| ATOM | 546 | O   | VAL | A | 85 | -1.573 | -4.163  | 26.594 | 1.000 | 24.70 |
| ATOM | 547 | N   | LYS | A | 86 | -1.270 | -5.081  | 24.590 | 1.000 | 22.80 |
| ATOM | 548 | CA  | LYS | A | 86 | -2.572 | -5.741  | 24.686 | 1.000 | 22.12 |
| ATOM | 549 | CB  | LYS | A | 86 | -3.307 | -5.564  | 23.347 | 1.000 | 31.33 |
| ATOM | 550 | CG  | LYS | A | 86 | -3.256 | -4.147  | 22.803 | 1.000 | 27.28 |
| ATOM | 551 | CD  | LYS | A | 86 | -3.691 | -4.077  | 21.352 | 1.000 | 33.19 |
| ATOM | 552 | CE  | LYS | A | 86 | -4.193 | -2.688  | 20.990 | 1.000 | 43.70 |
| ATOM | 553 | NZ  | LYS | A | 86 | -4.520 | -2.549  | 19.542 | 1.000 | 37.64 |
| ATOM | 554 | C   | LYS | A | 86 | -2.483 | -7.222  | 25.020 | 1.000 | 24.22 |
| ATOM | 555 | O   | LYS | A | 86 | -1.658 | -7.961  | 24.475 | 1.000 | 27.05 |
| ATOM | 556 | N   | LEU | A | 87 | -3.358 | -7.682  | 25.911 | 1.000 | 23.05 |
| ATOM | 557 | CA  | LEU | A | 87 | -3.530 | -9.107  | 26.143 | 1.000 | 23.37 |
| ATOM | 558 | CB  | LEU | A | 87 | -4.250 | -9.392  | 27.460 | 1.000 | 24.62 |
| ATOM | 559 | CG  | LEU | A | 87 | -3.733 | -8.696  | 28.711 | 1.000 | 27.34 |
| ATOM | 560 | CD1 | LEU | A | 87 | -4.614 | -9.032  | 29.904 | 1.000 | 20.48 |
| ATOM | 561 | CD2 | LEU | A | 87 | -2.284 | -9.078  | 28.973 | 1.000 | 32.54 |
| ATOM | 562 | C   | LEU | A | 87 | -4.360 | -9.720  | 25.020 | 1.000 | 26.94 |
| ATOM | 563 | O   | LEU | A | 87 | -5.318 | -9.094  | 24.555 | 1.000 | 38.77 |
| ATOM | 564 | N   | SER | A | 88 | -4.021 | -10.925 | 24.581 | 1.000 | 33.75 |
| ATOM | 565 | CA  | SER | A | 88 | -4.872 | -11.557 | 23.567 | 1.000 | 42.66 |
| ATOM | 566 | CB  | SER | A | 88 | -4.317 | -12.913 | 23.154 | 1.000 | 46.57 |
| ATOM | 567 | OG  | SER | A | 88 | -4.765 | -13.947 | 24.014 | 1.000 | 59.78 |
| ATOM | 568 | C   | SER | A | 88 | -6.292 | -11.680 | 24.113 | 1.000 | 52.63 |
| ATOM | 569 | O   | SER | A | 88 | -6.499 | -11.777 | 25.325 | 1.000 | 40.47 |
| ATOM | 570 | N   | ASN | A | 89 | -7.274 | -11.656 | 23.225 | 1.000 | 65.95 |
| ATOM | 571 | CA  | ASN | A | 89 | -8.680 | -11.790 | 23.586 | 1.000 | 71.68 |

**FIGURE 17**

|      |     |     |     |   |    |         |         |        |       |        |
|------|-----|-----|-----|---|----|---------|---------|--------|-------|--------|
| ATOM | 572 | CB  | ASN | A | 89 | -9.528  | -11.132 | 22.496 | 1.000 | 75.26  |
| ATOM | 573 | CG  | ASN | A | 89 | -8.793  | -11.244 | 21.163 | 1.000 | 78.86  |
| ATOM | 574 | OD1 | ASN | A | 89 | -7.806  | -10.546 | 20.946 | 1.000 | 71.99  |
| ATOM | 575 | ND2 | ASN | A | 89 | -9.271  | -12.122 | 20.293 | 1.000 | 90.92  |
| ATOM | 576 | C   | ASN | A | 89 | -9.057  | -13.256 | 23.738 | 1.000 | 79.05  |
| ATOM | 577 | O   | ASN | A | 89 | -8.808  | -14.039 | 22.811 | 1.000 | 73.71  |
| ATOM | 578 | N   | VAL | A | 90 | -9.633  | -13.639 | 24.875 | 1.000 | 87.92  |
| ATOM | 579 | CA  | VAL | A | 90 | -9.929  | -15.052 | 25.128 | 1.000 | 94.68  |
| ATOM | 580 | CB  | VAL | A | 90 | -8.920  | -15.629 | 26.140 | 1.000 | 89.31  |
| ATOM | 581 | CG1 | VAL | A | 90 | -7.494  | -15.497 | 25.590 | 1.000 | 54.27  |
| ATOM | 582 | CG2 | VAL | A | 90 | -9.031  | -14.923 | 27.491 | 1.000 | 100.28 |
| ATOM | 583 | C   | VAL | A | 90 | -11.354 | -15.293 | 25.619 | 1.000 | 102.19 |
| ATOM | 584 | O   | VAL | A | 90 | -12.315 | -14.798 | 25.014 | 1.000 | 100.56 |
| ATOM | 585 | N   | ASP | A | 91 | -11.498 | -16.059 | 26.693 | 1.000 | 105.22 |
| ATOM | 586 | CA  | ASP | A | 91 | -12.783 | -16.447 | 27.271 | 1.000 | 108.70 |
| ATOM | 587 | CB  | ASP | A | 91 | -12.578 | -17.068 | 28.656 | 1.000 | 107.42 |
| ATOM | 588 | CG  | ASP | A | 91 | -13.530 | -18.205 | 28.939 | 1.000 | 106.43 |
| ATOM | 589 | OD1 | ASP | A | 91 | -13.926 | -18.900 | 27.974 | 1.000 | 113.61 |
| ATOM | 590 | OD2 | ASP | A | 91 | -13.894 | -18.413 | 30.116 | 1.000 | 86.41  |
| ATOM | 591 | C   | ASP | A | 91 | -13.743 | -15.268 | 27.371 | 1.000 | 115.28 |
| ATOM | 592 | O   | ASP | A | 91 | -13.390 | -14.223 | 27.924 | 1.000 | 126.76 |
| ATOM | 593 | N   | ASP | A | 92 | -14.952 | -15.429 | 26.834 | 1.000 | 116.43 |
| ATOM | 594 | CA  | ASP | A | 92 | -15.914 | -14.333 | 26.741 | 1.000 | 116.50 |
| ATOM | 595 | CB  | ASP | A | 92 | -16.500 | -13.952 | 28.090 | 1.000 | 111.11 |
| ATOM | 596 | CG  | ASP | A | 92 | -17.029 | -15.093 | 28.929 | 1.000 | 103.39 |
| ATOM | 597 | OD1 | ASP | A | 92 | -17.835 | -15.908 | 28.441 | 1.000 | 70.91  |
| ATOM | 598 | OD2 | ASP | A | 92 | -16.639 | -15.180 | 30.116 | 1.000 | 105.06 |
| ATOM | 599 | C   | ASP | A | 92 | -15.224 | -13.122 | 26.103 | 1.000 | 121.44 |
| ATOM | 600 | O   | ASP | A | 92 | -14.846 | -13.211 | 24.935 | 1.000 | 119.15 |
| ATOM | 601 | N   | ASP | A | 93 | -15.077 | -12.068 | 26.886 | 1.000 | 124.91 |
| ATOM | 602 | CA  | ASP | A | 93 | -14.260 | -10.887 | 26.698 | 1.000 | 127.04 |
| ATOM | 603 | CB  | ASP | A | 93 | -13.201 | -11.126 | 25.615 | 1.000 | 127.70 |
| ATOM | 604 | CG  | ASP | A | 93 | -13.710 | -10.960 | 24.174 | 1.000 | 128.89 |
| ATOM | 605 | OD1 | ASP | A | 93 | -14.877 | -11.323 | 23.869 | 1.000 | 136.07 |
| ATOM | 606 | OD2 | ASP | A | 93 | -12.928 | -10.464 | 23.315 | 1.000 | 126.93 |
| ATOM | 607 | C   | ASP | A | 93 | -15.055 | -9.617  | 26.384 | 1.000 | 125.66 |
| ATOM | 608 | O   | ASP | A | 93 | -15.775 | -9.536  | 25.388 | 1.000 | 112.27 |
| ATOM | 609 | N   | PRO | A | 94 | -14.884 | -8.640  | 27.272 | 1.000 | 123.81 |
| ATOM | 610 | CA  | PRO | A | 94 | -15.331 | -7.253  | 27.126 | 1.000 | 114.77 |
| ATOM | 611 | CB  | PRO | A | 94 | -15.751 | -6.908  | 28.554 | 1.000 | 118.39 |
| ATOM | 612 | CG  | PRO | A | 94 | -14.893 | -7.760  | 29.440 | 1.000 | 121.09 |
| ATOM | 613 | CD  | PRO | A | 94 | -14.224 | -8.799  | 28.586 | 1.000 | 123.81 |
| ATOM | 614 | C   | PRO | A | 94 | -14.172 | -6.360  | 26.685 | 1.000 | 99.08  |
| ATOM | 615 | O   | PRO | A | 94 | -14.080 | -5.961  | 25.527 | 1.000 | 69.91  |
| ATOM | 616 | N   | CYS | A | 95 | -13.294 | -6.071  | 27.635 | 1.000 | 91.61  |
| ATOM | 617 | CA  | CYS | A | 95 | -11.981 | -5.485  | 27.441 | 1.000 | 80.21  |
| ATOM | 618 | CB  | CYS | A | 95 | -11.883 | -4.014  | 27.797 | 1.000 | 80.05  |
| ATOM | 619 | SG  | CYS | A | 95 | -10.319 | -3.186  | 27.438 | 1.000 | 75.64  |
| ATOM | 620 | C   | CYS | A | 95 | -10.991 | -6.285  | 28.303 | 1.000 | 67.30  |
| ATOM | 621 | O   | CYS | A | 95 | -10.299 | -5.735  | 29.149 | 1.000 | 48.15  |
| ATOM | 622 | N   | SER | A | 96 | -10.993 | -7.580  | 28.030 | 1.000 | 62.04  |
| ATOM | 623 | CA  | SER | A | 96 | -10.102 | -8.548  | 28.645 | 1.000 | 49.24  |

FIGURE 18

|      |     |     |     |   |     |         |         |        |       |       |
|------|-----|-----|-----|---|-----|---------|---------|--------|-------|-------|
| ATOM | 624 | CB  | SER | A | 96  | -10.644 | -9.959  | 28.392 | 1.000 | 47.34 |
| ATOM | 625 | OG  | SER | A | 96  | -10.772 | -10.165 | 26.989 | 1.000 | 35.99 |
| ATOM | 626 | C   | SER | A | 96  | -8.689  | -8.404  | 28.091 | 1.000 | 40.83 |
| ATOM | 627 | O   | SER | A | 96  | -7.762  | -9.091  | 28.530 | 1.000 | 43.79 |
| ATOM | 628 | N   | ASP | A | 97  | -8.519  | -7.503  | 27.119 | 1.000 | 33.54 |
| ATOM | 629 | CA  | ASP | A | 97  | -7.200  | -7.260  | 26.543 | 1.000 | 26.97 |
| ATOM | 630 | CB  | ASP | A | 97  | -7.333  | -6.817  | 25.088 | 1.000 | 24.79 |
| ATOM | 631 | CG  | ASP | A | 97  | -7.611  | -5.353  | 24.842 | 1.000 | 31.75 |
| ATOM | 632 | OD1 | ASP | A | 97  | -7.973  | -4.566  | 25.740 | 1.000 | 34.88 |
| ATOM | 633 | OD2 | ASP | A | 97  | -7.473  | -4.920  | 23.667 | 1.000 | 32.46 |
| ATOM | 634 | C   | ASP | A | 97  | -6.406  | -6.227  | 27.331 | 1.000 | 19.31 |
| ATOM | 635 | O   | ASP | A | 97  | -5.239  | -6.008  | 27.001 | 1.000 | 32.90 |
| ATOM | 636 | N   | TYR | A | 98  | -7.001  | -5.563  | 28.319 | 1.000 | 21.87 |
| ATOM | 637 | CA  | TYR | A | 98  | -6.317  | -4.446  | 28.958 | 1.000 | 24.52 |
| ATOM | 638 | CB  | TYR | A | 98  | -7.294  | -3.441  | 29.604 | 1.000 | 22.29 |
| ATOM | 639 | CG  | TYR | A | 98  | -6.556  | -2.288  | 30.277 | 1.000 | 21.76 |
| ATOM | 640 | CD1 | TYR | A | 98  | -6.012  | -1.275  | 29.489 | 1.000 | 23.46 |
| ATOM | 641 | CE1 | TYR | A | 98  | -5.324  | -0.202  | 30.044 | 1.000 | 12.80 |
| ATOM | 642 | CZ  | TYR | A | 98  | -5.184  | -0.152  | 31.415 | 1.000 | 16.57 |
| ATOM | 643 | OH  | TYR | A | 98  | -4.516  | 0.900   | 32.001 | 1.000 | 20.04 |
| ATOM | 644 | CE2 | TYR | A | 98  | -5.710  | -1.138  | 32.234 | 1.000 | 21.65 |
| ATOM | 645 | CD2 | TYR | A | 98  | -6.388  | -2.192  | 31.652 | 1.000 | 22.47 |
| ATOM | 646 | C   | TYR | A | 98  | -5.329  | -4.852  | 30.045 | 1.000 | 23.39 |
| ATOM | 647 | O   | TYR | A | 98  | -5.609  | -5.609  | 30.964 | 1.000 | 28.32 |
| ATOM | 648 | N   | ILE | A | 99  | -4.143  | -4.250  | 29.978 | 1.000 | 19.82 |
| ATOM | 649 | CA  | ILE | A | 99  | -3.247  | -4.242  | 31.130 | 1.000 | 21.08 |
| ATOM | 650 | CB  | ILE | A | 99  | -2.185  | -5.354  | 31.091 | 1.000 | 21.45 |
| ATOM | 651 | CG1 | ILE | A | 99  | -1.169  | -5.304  | 32.224 | 1.000 | 13.12 |
| ATOM | 652 | CD1 | ILE | A | 99  | -0.466  | -6.601  | 32.573 | 1.000 | 15.73 |
| ATOM | 653 | CG2 | ILE | A | 99  | -1.481  | -5.344  | 29.737 | 1.000 | 24.91 |
| ATOM | 654 | C   | ILE | A | 99  | -2.593  | -2.867  | 31.218 | 1.000 | 17.86 |
| ATOM | 655 | O   | ILE | A | 99  | -2.362  | -2.161  | 30.235 | 1.000 | 23.00 |
| ATOM | 656 | N   | ASN | A | 100 | -2.271  | -2.426  | 32.429 | 1.000 | 17.97 |
| ATOM | 657 | CA  | ASN | A | 100 | -1.523  | -1.168  | 32.506 | 1.000 | 16.53 |
| ATOM | 658 | CB  | ASN | A | 100 | -1.696  | -0.583  | 33.904 | 1.000 | 15.17 |
| ATOM | 659 | CG  | ASN | A | 100 | -1.169  | 0.837   | 33.940 | 1.000 | 17.63 |
| ATOM | 660 | OD1 | ASN | A | 100 | -0.087  | 1.081   | 33.409 | 1.000 | 19.68 |
| ATOM | 661 | ND2 | ASN | A | 100 | -1.931  | 1.727   | 34.566 | 1.000 | 19.64 |
| ATOM | 662 | C   | ASN | A | 100 | -0.064  | -1.408  | 32.144 | 1.000 | 20.69 |
| ATOM | 663 | O   | ASN | A | 100 | 0.784   | -1.727  | 32.977 | 1.000 | 13.39 |
| ATOM | 664 | N   | ALA | A | 101 | 0.246   | -1.268  | 30.851 | 1.000 | 11.73 |
| ATOM | 665 | CA  | ALA | A | 101 | 1.586   | -1.586  | 30.370 | 1.000 | 13.46 |
| ATOM | 666 | CB  | ALA | A | 101 | 1.737   | -3.096  | 30.235 | 1.000 | 16.17 |
| ATOM | 667 | C   | ALA | A | 101 | 1.842   | -0.930  | 29.026 | 1.000 | 14.30 |
| ATOM | 668 | O   | ALA | A | 101 | 0.883   | -0.739  | 28.277 | 1.000 | 15.61 |
| ATOM | 669 | N   | SER | A | 102 | 3.088   | -0.603  | 28.708 | 1.000 | 17.77 |
| ATOM | 670 | CA  | SER | A | 102 | 3.385   | 0.102   | 27.472 | 1.000 | 18.13 |
| ATOM | 671 | CB  | SER | A | 102 | 3.627   | 1.593   | 27.759 | 1.000 | 13.36 |
| ATOM | 672 | OG  | SER | A | 102 | 2.735   | 2.076   | 28.738 | 1.000 | 20.39 |
| ATOM | 673 | C   | SER | A | 102 | 4.623   | -0.444  | 26.786 | 1.000 | 23.90 |
| ATOM | 674 | O   | SER | A | 102 | 5.568   | -0.832  | 27.475 | 1.000 | 22.19 |
| ATOM | 675 | N   | TYR | A | 103 | 4.639   | -0.454  | 25.452 | 1.000 | 16.79 |

**FIGURE 19**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 676 | CA  | TYR | A | 103 | 5.871  | -0.877 | 24.793 | 1.000 | 10.43 |
| ATOM | 677 | CB  | TYR | A | 103 | 5.619  | -1.287 | 23.347 | 1.000 | 16.27 |
| ATOM | 678 | CG  | TYR | A | 103 | 4.840  | -2.567 | 23.157 | 1.000 | 15.11 |
| ATOM | 679 | CD1 | TYR | A | 103 | 5.421  | -3.802 | 23.412 | 1.000 | 18.80 |
| ATOM | 680 | CE1 | TYR | A | 103 | 4.704  | -4.978 | 23.232 | 1.000 | 22.75 |
| ATOM | 681 | CZ  | TYR | A | 103 | 3.396  | -4.922 | 22.798 | 1.000 | 19.98 |
| ATOM | 682 | OH  | TYR | A | 103 | 2.689  | -6.094 | 22.625 | 1.000 | 16.85 |
| ATOM | 683 | CE2 | TYR | A | 103 | 2.797  | -3.704 | 22.536 | 1.000 | 14.29 |
| ATOM | 684 | CD2 | TYR | A | 103 | 3.517  | -2.540 | 22.714 | 1.000 | 12.99 |
| ATOM | 685 | C   | TYR | A | 103 | 6.847  | 0.293  | 24.853 | 1.000 | 19.42 |
| ATOM | 686 | O   | TYR | A | 103 | 6.398  | 1.440  | 24.787 | 1.000 | 21.35 |
| ATOM | 687 | N   | ILE | A | 104 | 8.143  | 0.039  | 24.983 | 1.000 | 20.28 |
| ATOM | 688 | CA  | ILE | A | 104 | 9.090  | 1.151  | 25.068 | 1.000 | 18.75 |
| ATOM | 689 | CB  | ILE | A | 104 | 9.522  | 1.444  | 26.516 | 1.000 | 25.72 |
| ATOM | 690 | CG1 | ILE | A | 104 | 8.372  | 1.673  | 27.507 | 1.000 | 19.54 |
| ATOM | 691 | CD1 | ILE | A | 104 | 7.657  | 2.991  | 27.243 | 1.000 | 24.18 |
| ATOM | 692 | CG2 | ILE | A | 104 | 10.466 | 2.640  | 26.556 | 1.000 | 25.08 |
| ATOM | 693 | C   | ILE | A | 104 | 10.321 | 0.843  | 24.229 | 1.000 | 18.91 |
| ATOM | 694 | O   | ILE | A | 104 | 10.899 | -0.236 | 24.356 | 1.000 | 21.99 |
| ATOM | 695 | N   | PRO | A | 105 | 10.719 | 1.777  | 23.376 | 1.000 | 25.40 |
| ATOM | 696 | CA  | PRO | A | 105 | 11.854 | 1.513  | 22.482 | 1.000 | 23.49 |
| ATOM | 697 | CB  | PRO | A | 105 | 11.761 | 2.641  | 21.457 | 1.000 | 25.41 |
| ATOM | 698 | CG  | PRO | A | 105 | 11.030 | 3.747  | 22.133 | 1.000 | 26.30 |
| ATOM | 699 | CD  | PRO | A | 105 | 10.166 | 3.121  | 23.187 | 1.000 | 24.38 |
| ATOM | 700 | C   | PRO | A | 105 | 13.165 | 1.602  | 23.249 | 1.000 | 24.84 |
| ATOM | 701 | O   | PRO | A | 105 | 13.255 | 2.321  | 24.246 | 1.000 | 19.70 |
| ATOM | 702 | N   | GLY | A | 106 | 14.176 | 0.872  | 22.788 | 1.000 | 21.42 |
| ATOM | 703 | CA  | GLY | A | 106 | 15.485 | 1.020  | 23.423 | 1.000 | 28.59 |
| ATOM | 704 | C   | GLY | A | 106 | 16.527 | 1.498  | 22.425 | 1.000 | 30.55 |
| ATOM | 705 | O   | GLY | A | 106 | 16.222 | 2.089  | 21.395 | 1.000 | 20.21 |
| ATOM | 706 | N   | ASN | A | 107 | 17.796 | 1.244  | 22.710 | 1.000 | 32.09 |
| ATOM | 707 | CA  | ASN | A | 107 | 18.884 | 1.677  | 21.850 | 1.000 | 26.56 |
| ATOM | 708 | CB  | ASN | A | 107 | 20.219 | 1.386  | 22.552 | 1.000 | 28.73 |
| ATOM | 709 | CG  | ASN | A | 107 | 20.932 | 2.668  | 22.930 | 1.000 | 36.73 |
| ATOM | 710 | OD1 | ASN | A | 107 | 20.436 | 3.454  | 23.736 | 1.000 | 67.71 |
| ATOM | 711 | ND2 | ASN | A | 107 | 22.095 | 2.891  | 22.331 | 1.000 | 51.19 |
| ATOM | 712 | C   | ASN | A | 107 | 18.828 | 0.985  | 20.497 | 1.000 | 33.29 |
| ATOM | 713 | O   | ASN | A | 107 | 19.161 | 1.589  | 19.469 | 1.000 | 31.37 |
| ATOM | 714 | N   | ASN | A | 108 | 18.394 | -0.282 | 20.495 | 1.000 | 25.02 |
| ATOM | 715 | CA  | ASN | A | 108 | 18.476 | -1.030 | 19.241 | 1.000 | 37.28 |
| ATOM | 716 | CB  | ASN | A | 108 | 19.377 | -2.255 | 19.480 | 1.000 | 49.51 |
| ATOM | 717 | CG  | ASN | A | 108 | 20.794 | -1.843 | 19.847 | 1.000 | 47.25 |
| ATOM | 718 | OD1 | ASN | A | 108 | 21.555 | -1.301 | 19.041 | 1.000 | 51.78 |
| ATOM | 719 | ND2 | ASN | A | 108 | 21.149 | -2.103 | 21.097 | 1.000 | 32.89 |
| ATOM | 720 | C   | ASN | A | 108 | 17.157 | -1.472 | 18.642 | 1.000 | 41.66 |
| ATOM | 721 | O   | ASN | A | 108 | 17.148 | -1.922 | 17.485 | 1.000 | 47.43 |
| ATOM | 722 | N   | PHE | A | 109 | 16.007 | -1.389 | 19.306 | 1.000 | 28.44 |
| ATOM | 723 | CA  | PHE | A | 109 | 14.782 | -1.693 | 18.557 | 1.000 | 26.26 |
| ATOM | 724 | CB  | PHE | A | 109 | 14.575 | -3.179 | 18.334 | 1.000 | 25.58 |
| ATOM | 725 | CG  | PHE | A | 109 | 14.889 | -4.154 | 19.423 | 1.000 | 33.48 |
| ATOM | 726 | CD1 | PHE | A | 109 | 13.866 | -4.796 | 20.113 | 1.000 | 34.64 |
| ATOM | 727 | CE1 | PHE | A | 109 | 14.130 | -5.705 | 21.121 | 1.000 | 41.36 |

**FIGURE 20**



|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 728 | CZ  | PHE | A | 109 | 15.442 | -5.997 | 21.459 | 1.000 | 37.10 |
| ATOM | 729 | CE2 | PHE | A | 109 | 16.469 | -5.365 | 20.782 | 1.000 | 39.85 |
| ATOM | 730 | CD2 | PHE | A | 109 | 16.198 | -4.452 | 19.778 | 1.000 | 33.66 |
| ATOM | 731 | C   | PHE | A | 109 | 13.572 | -1.059 | 19.243 | 1.000 | 30.59 |
| ATOM | 732 | O   | PHE | A | 109 | 13.663 | -0.571 | 20.375 | 1.000 | 28.48 |
| ATOM | 733 | N   | ARG | A | 110 | 12.446 | -1.068 | 18.531 | 1.000 | 21.36 |
| ATOM | 734 | CA  | ARG | A | 110 | 11.262 | -0.340 | 18.981 | 1.000 | 27.72 |
| ATOM | 735 | CB  | ARG | A | 110 | 10.239 | -0.271 | 17.833 | 1.000 | 27.18 |
| ATOM | 736 | CG  | ARG | A | 110 | 10.751 | 0.480  | 16.614 | 1.000 | 42.55 |
| ATOM | 737 | CD  | ARG | A | 110 | 10.188 | 1.893  | 16.543 | 1.000 | 49.91 |
| ATOM | 738 | NE  | ARG | A | 110 | 11.080 | 2.835  | 17.214 | 1.000 | 61.23 |
| ATOM | 739 | CZ  | ARG | A | 110 | 10.772 | 4.078  | 17.551 | 1.000 | 65.49 |
| ATOM | 740 | NH1 | ARG | A | 110 | 9.569  | 4.569  | 17.287 | 1.000 | 60.40 |
| ATOM | 741 | NH2 | ARG | A | 110 | 11.681 | 4.823  | 18.164 | 1.000 | 70.08 |
| ATOM | 742 | C   | ARG | A | 110 | 10.581 | -0.929 | 20.206 | 1.000 | 31.32 |
| ATOM | 743 | O   | ARG | A | 110 | 10.063 | -0.191 | 21.048 | 1.000 | 19.57 |
| ATOM | 744 | N   | ARG | A | 111 | 10.536 | -2.256 | 20.315 | 1.000 | 31.03 |
| ATOM | 745 | CA  | ARG | A | 111 | 9.825  | -2.858 | 21.447 | 1.000 | 28.45 |
| ATOM | 746 | CB  | ARG | A | 111 | 8.752  | -3.826 | 20.971 | 1.000 | 24.30 |
| ATOM | 747 | CG  | ARG | A | 111 | 7.678  | -3.274 | 20.054 | 1.000 | 26.60 |
| ATOM | 748 | CD  | ARG | A | 111 | 6.895  | -4.443 | 19.432 | 1.000 | 26.88 |
| ATOM | 749 | NE  | ARG | A | 111 | 5.494  | -4.083 | 19.259 | 1.000 | 39.04 |
| ATOM | 750 | CZ  | ARG | A | 111 | 4.427  | -4.851 | 19.403 | 1.000 | 38.77 |
| ATOM | 751 | NH1 | ARG | A | 111 | 4.532  | -6.128 | 19.745 | 1.000 | 39.25 |
| ATOM | 752 | NH2 | ARG | A | 111 | 3.226  | -4.319 | 19.199 | 1.000 | 38.01 |
| ATOM | 753 | C   | ARG | A | 111 | 10.821 | -3.575 | 22.352 | 1.000 | 27.13 |
| ATOM | 754 | O   | ARG | A | 111 | 10.716 | -4.761 | 22.672 | 1.000 | 22.92 |
| ATOM | 755 | N   | GLU | A | 112 | 11.827 | -2.801 | 22.753 | 1.000 | 24.46 |
| ATOM | 756 | CA  | GLU | A | 112 | 12.921 | -3.388 | 23.527 | 1.000 | 20.04 |
| ATOM | 757 | CB  | GLU | A | 112 | 14.147 | -2.484 | 23.425 | 1.000 | 26.41 |
| ATOM | 758 | CG  | GLU | A | 112 | 15.469 | -3.181 | 23.658 | 1.000 | 27.73 |
| ATOM | 759 | CD  | GLU | A | 112 | 16.662 | -2.423 | 23.112 | 1.000 | 26.53 |
| ATOM | 760 | OE1 | GLU | A | 112 | 17.767 | -2.676 | 23.628 | 1.000 | 22.28 |
| ATOM | 761 | OE2 | GLU | A | 112 | 16.520 | -1.592 | 22.191 | 1.000 | 24.96 |
| ATOM | 762 | C   | GLU | A | 112 | 12.523 | -3.597 | 24.976 | 1.000 | 14.90 |
| ATOM | 763 | O   | GLU | A | 112 | 13.092 | -4.442 | 25.668 | 1.000 | 19.62 |
| ATOM | 764 | N   | TYR | A | 113 | 11.540 | -2.823 | 25.426 | 1.000 | 12.89 |
| ATOM | 765 | CA  | TYR | A | 113 | 11.084 | -2.956 | 26.807 | 1.000 | 16.51 |
| ATOM | 766 | CB  | TYR | A | 113 | 11.619 | -1.873 | 27.733 | 1.000 | 20.74 |
| ATOM | 767 | CG  | TYR | A | 113 | 13.078 | -1.515 | 27.619 | 1.000 | 26.13 |
| ATOM | 768 | CD1 | TYR | A | 113 | 13.516 | -0.557 | 26.718 | 1.000 | 18.47 |
| ATOM | 769 | CE1 | TYR | A | 113 | 14.856 | -0.215 | 26.600 | 1.000 | 15.41 |
| ATOM | 770 | CZ  | TYR | A | 113 | 15.762 | -0.861 | 27.419 | 1.000 | 20.13 |
| ATOM | 771 | OH  | TYR | A | 113 | 17.101 | -0.557 | 27.351 | 1.000 | 18.27 |
| ATOM | 772 | CE2 | TYR | A | 113 | 15.348 | -1.814 | 28.327 | 1.000 | 21.37 |
| ATOM | 773 | CD2 | TYR | A | 113 | 14.015 | -2.150 | 28.439 | 1.000 | 19.35 |
| ATOM | 774 | C   | TYR | A | 113 | 9.561  | -2.892 | 26.883 | 1.000 | 12.89 |
| ATOM | 775 | O   | TYR | A | 113 | 8.890  | -2.269 | 26.069 | 1.000 | 17.48 |
| ATOM | 776 | N   | ILE | A | 114 | 9.052  | -3.550 | 27.919 | 1.000 | 15.07 |
| ATOM | 777 | CA  | ILE | A | 114 | 7.656  | -3.353 | 28.290 | 1.000 | 16.69 |
| ATOM | 778 | CB  | ILE | A | 114 | 6.820  | -4.639 | 28.237 | 1.000 | 20.07 |
| ATOM | 779 | CG1 | ILE | A | 114 | 6.471  | -5.095 | 26.816 | 1.000 | 12.15 |

**FIGURE 21**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 780 | CD1 | ILE | A | 114 | 6.039  | -6.546 | 26.725 | 1.000 | 8.94  |
| ATOM | 781 | CG2 | ILE | A | 114 | 5.565  | -4.473 | 29.088 | 1.000 | 8.30  |
| ATOM | 782 | C   | ILE | A | 114 | 7.694  | -2.763 | 29.700 | 1.000 | 14.06 |
| ATOM | 783 | O   | ILE | A | 114 | 8.303  | -3.348 | 30.598 | 1.000 | 21.26 |
| ATOM | 784 | N   | VAL | A | 115 | 7.089  | -1.596 | 29.869 | 1.000 | 14.01 |
| ATOM | 785 | CA  | VAL | A | 115 | 7.062  | -0.937 | 31.174 | 1.000 | 13.47 |
| ATOM | 786 | CB  | VAL | A | 115 | 7.364  | 0.562  | 31.033 | 1.000 | 21.33 |
| ATOM | 787 | CG1 | VAL | A | 115 | 6.907  | 1.314  | 32.276 | 1.000 | 36.92 |
| ATOM | 788 | CG2 | VAL | A | 115 | 8.848  | 0.796  | 30.787 | 1.000 | 22.96 |
| ATOM | 789 | C   | VAL | A | 115 | 5.679  | -1.158 | 31.777 | 1.000 | 17.22 |
| ATOM | 790 | O   | VAL | A | 115 | 4.690  | -0.963 | 31.064 | 1.000 | 14.66 |
| ATOM | 791 | N   | THR | A | 116 | 5.582  | -1.561 | 33.041 | 1.000 | 12.85 |
| ATOM | 792 | CA  | THR | A | 116 | 4.240  | -1.763 | 33.594 | 1.000 | 13.54 |
| ATOM | 793 | CB  | THR | A | 116 | 3.847  | -3.242 | 33.400 | 1.000 | 21.30 |
| ATOM | 794 | OG1 | THR | A | 116 | 2.453  | -3.453 | 33.671 | 1.000 | 12.82 |
| ATOM | 795 | CG2 | THR | A | 116 | 4.622  | -4.140 | 34.364 | 1.000 | 10.46 |
| ATOM | 796 | C   | THR | A | 116 | 4.203  | -1.329 | 35.050 | 1.000 | 19.71 |
| ATOM | 797 | O   | THR | A | 116 | 5.232  | -0.961 | 35.629 | 1.000 | 17.41 |
| ATOM | 798 | N   | GLN | A | 117 | 3.030  | -1.346 | 35.671 | 1.000 | 15.37 |
| ATOM | 799 | CA  | GLN | A | 117 | 2.879  | -0.940 | 37.068 | 1.000 | 16.82 |
| ATOM | 800 | CB  | GLN | A | 117 | 1.431  | -0.504 | 37.325 | 1.000 | 15.09 |
| ATOM | 801 | CG  | GLN | A | 117 | 0.408  | -1.602 | 37.048 | 1.000 | 19.18 |
| ATOM | 802 | CD  | GLN | A | 117 | -1.027 | -1.187 | 37.299 | 1.000 | 20.69 |
| ATOM | 803 | OE1 | GLN | A | 117 | -1.353 | -0.007 | 37.405 | 1.000 | 25.69 |
| ATOM | 804 | NE2 | GLN | A | 117 | -1.921 | -2.158 | 37.408 | 1.000 | 18.66 |
| ATOM | 805 | C   | GLN | A | 117 | 3.256  | -2.108 | 37.959 | 1.000 | 19.79 |
| ATOM | 806 | O   | GLN | A | 117 | 3.305  | -3.228 | 37.431 | 1.000 | 16.87 |
| ATOM | 807 | N   | GLY | A | 118 | 3.513  | -1.947 | 39.253 | 1.000 | 17.49 |
| ATOM | 808 | CA  | GLY | A | 118 | 3.594  | -3.168 | 40.078 | 1.000 | 15.99 |
| ATOM | 809 | C   | GLY | A | 118 | 2.238  | -3.855 | 40.061 | 1.000 | 17.56 |
| ATOM | 810 | O   | GLY | A | 118 | 1.217  | -3.179 | 40.257 | 1.000 | 18.31 |
| ATOM | 811 | N   | PRO | A | 119 | 2.182  | -5.164 | 39.834 | 1.000 | 24.40 |
| ATOM | 812 | CA  | PRO | A | 119 | 0.885  | -5.845 | 39.699 | 1.000 | 30.48 |
| ATOM | 813 | CB  | PRO | A | 119 | 1.272  | -7.296 | 39.388 | 1.000 | 31.82 |
| ATOM | 814 | CG  | PRO | A | 119 | 2.683  | -7.227 | 38.899 | 1.000 | 29.01 |
| ATOM | 815 | CD  | PRO | A | 119 | 3.310  | -6.102 | 39.686 | 1.000 | 21.75 |
| ATOM | 816 | C   | PRO | A | 119 | 0.033  | -5.781 | 40.966 | 1.000 | 34.89 |
| ATOM | 817 | O   | PRO | A | 119 | 0.531  | -5.756 | 42.091 | 1.000 | 19.13 |
| ATOM | 818 | N   | LEU | A | 120 | -1.288 | -5.753 | 40.778 | 1.000 | 30.42 |
| ATOM | 819 | CA  | LEU | A | 120 | -2.231 | -5.801 | 41.886 | 1.000 | 18.88 |
| ATOM | 820 | CB  | LEU | A | 120 | -3.467 | -4.949 | 41.613 | 1.000 | 22.55 |
| ATOM | 821 | CG  | LEU | A | 120 | -3.264 | -3.439 | 41.494 | 1.000 | 24.74 |
| ATOM | 822 | CD1 | LEU | A | 120 | -4.202 | -2.849 | 40.458 | 1.000 | 19.55 |
| ATOM | 823 | CD2 | LEU | A | 120 | -3.482 | -2.766 | 42.842 | 1.000 | 27.98 |
| ATOM | 824 | C   | LEU | A | 120 | -2.690 | -7.241 | 42.099 | 1.000 | 25.27 |
| ATOM | 825 | O   | LEU | A | 120 | -2.588 | -8.006 | 41.139 | 1.000 | 22.48 |
| ATOM | 826 | N   | PRO | A | 121 | -3.160 | -7.550 | 43.298 | 1.000 | 32.56 |
| ATOM | 827 | CA  | PRO | A | 121 | -3.719 | -8.872 | 43.596 | 1.000 | 22.33 |
| ATOM | 828 | CB  | PRO | A | 121 | -4.528 | -8.621 | 44.871 | 1.000 | 23.26 |
| ATOM | 829 | CG  | PRO | A | 121 | -3.777 | -7.531 | 45.557 | 1.000 | 29.77 |
| ATOM | 830 | CD  | PRO | A | 121 | -3.184 | -6.660 | 44.477 | 1.000 | 30.93 |
| ATOM | 831 | C   | PRO | A | 121 | -4.638 | -9.339 | 42.476 | 1.000 | 23.80 |

**FIGURE 22**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |         |        |       |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 832 | O   | PRO | A | 121 | -4.596 | -10.483 | 42.026 | 1.000 | 34.64 |
| ATOM | 833 | N   | GLY | A | 122 | -5.453 | -8.405  | 41.983 | 1.000 | 24.62 |
| ATOM | 834 | CA  | GLY | A | 122 | -6.344 | -8.742  | 40.887 | 1.000 | 23.65 |
| ATOM | 835 | C   | GLY | A | 122 | -5.751 | -8.605  | 39.505 | 1.000 | 23.11 |
| ATOM | 836 | O   | GLY | A | 122 | -6.478 | -8.836  | 38.533 | 1.000 | 28.12 |
| ATOM | 837 | N   | THR | A | 123 | -4.480 | -8.246  | 39.320 | 1.000 | 20.65 |
| ATOM | 838 | CA  | THR | A | 123 | -3.939 | -8.167  | 37.962 | 1.000 | 21.61 |
| ATOM | 839 | CB  | THR | A | 123 | -3.544 | -6.732  | 37.551 | 1.000 | 26.10 |
| ATOM | 840 | OG1 | THR | A | 123 | -2.505 | -6.195  | 38.380 | 1.000 | 23.39 |
| ATOM | 841 | CG2 | THR | A | 123 | -4.762 | -5.828  | 37.710 | 1.000 | 18.68 |
| ATOM | 842 | C   | THR | A | 123 | -2.713 | -9.052  | 37.765 | 1.000 | 24.76 |
| ATOM | 843 | O   | THR | A | 123 | -2.184 | -9.097  | 36.653 | 1.000 | 25.68 |
| ATOM | 844 | N   | LYS | A | 124 | -2.249 | -9.744  | 38.806 | 1.000 | 23.64 |
| ATOM | 845 | CA  | LYS | A | 124 | -1.015 | -10.520 | 38.633 | 1.000 | 29.85 |
| ATOM | 846 | CB  | LYS | A | 124 | -0.485 | -10.990 | 39.979 | 1.000 | 33.93 |
| ATOM | 847 | CG  | LYS | A | 124 | -1.476 | -11.566 | 40.964 | 1.000 | 33.84 |
| ATOM | 848 | CD  | LYS | A | 124 | -0.857 | -11.618 | 42.358 | 1.000 | 31.42 |
| ATOM | 849 | CE  | LYS | A | 124 | -1.630 | -12.583 | 43.246 | 1.000 | 29.23 |
| ATOM | 850 | NZ  | LYS | A | 124 | -0.899 | -12.844 | 44.518 | 1.000 | 57.02 |
| ATOM | 851 | C   | LYS | A | 124 | -1.209 | -11.674 | 37.656 | 1.000 | 25.22 |
| ATOM | 852 | O   | LYS | A | 124 | -0.283 | -12.089 | 36.954 | 1.000 | 23.70 |
| ATOM | 853 | N   | ASP | A | 125 | -2.412 | -12.221 | 37.545 | 1.000 | 18.28 |
| ATOM | 854 | CA  | ASP | A | 125 | -2.657 | -13.219 | 36.515 | 1.000 | 12.12 |
| ATOM | 855 | CB  | ASP | A | 125 | -4.097 | -13.722 | 36.640 | 1.000 | 22.43 |
| ATOM | 856 | CG  | ASP | A | 125 | -4.249 | -14.657 | 37.831 | 1.000 | 27.90 |
| ATOM | 857 | OD1 | ASP | A | 125 | -3.285 | -14.704 | 38.618 | 1.000 | 29.09 |
| ATOM | 858 | OD2 | ASP | A | 125 | -5.301 | -15.311 | 37.945 | 1.000 | 33.37 |
| ATOM | 859 | C   | ASP | A | 125 | -2.450 | -12.633 | 35.120 | 1.000 | 23.84 |
| ATOM | 860 | O   | ASP | A | 125 | -1.964 | -13.280 | 34.191 | 1.000 | 23.80 |
| ATOM | 861 | N   | ASP | A | 126 | -2.855 | -11.375 | 34.973 | 1.000 | 22.66 |
| ATOM | 862 | CA  | ASP | A | 126 | -2.745 | -10.631 | 33.732 | 1.000 | 16.52 |
| ATOM | 863 | CB  | ASP | A | 126 | -3.480 | -9.297  | 33.831 | 1.000 | 25.64 |
| ATOM | 864 | CG  | ASP | A | 126 | -4.972 | -9.394  | 33.608 | 1.000 | 41.42 |
| ATOM | 865 | OD1 | ASP | A | 126 | -5.419 | -10.439 | 33.084 | 1.000 | 47.26 |
| ATOM | 866 | OD2 | ASP | A | 126 | -5.703 | -8.435  | 33.953 | 1.000 | 43.25 |
| ATOM | 867 | C   | ASP | A | 126 | -1.274 | -10.385 | 33.422 | 1.000 | 17.37 |
| ATOM | 868 | O   | ASP | A | 126 | -0.798 | -10.492 | 32.297 | 1.000 | 16.89 |
| ATOM | 869 | N   | PHE | A | 127 | -0.544 | -10.017 | 34.473 | 1.000 | 17.74 |
| ATOM | 870 | CA  | PHE | A | 127 | 0.871  | -9.707  | 34.284 | 1.000 | 21.41 |
| ATOM | 871 | CB  | PHE | A | 127 | 1.493  | -9.263  | 35.604 | 1.000 | 21.46 |
| ATOM | 872 | CG  | PHE | A | 127 | 3.004  | -9.193  | 35.632 | 1.000 | 22.78 |
| ATOM | 873 | CD1 | PHE | A | 127 | 3.643  | -8.020  | 35.266 | 1.000 | 12.05 |
| ATOM | 874 | CE1 | PHE | A | 127 | 5.024  | -7.924  | 35.292 | 1.000 | 16.72 |
| ATOM | 875 | CZ  | PHE | A | 127 | 5.790  | -9.004  | 35.682 | 1.000 | 21.66 |
| ATOM | 876 | CE2 | PHE | A | 127 | 5.172  | -10.189 | 36.044 | 1.000 | 19.24 |
| ATOM | 877 | CD2 | PHE | A | 127 | 3.794  | -10.266 | 36.036 | 1.000 | 18.50 |
| ATOM | 878 | C   | PHE | A | 127 | 1.578  | -10.931 | 33.700 | 1.000 | 25.45 |
| ATOM | 879 | O   | PHE | A | 127 | 2.374  | -10.786 | 32.784 | 1.000 | 21.87 |
| ATOM | 880 | N   | TRP | A | 128 | 1.280  | -12.107 | 34.243 | 1.000 | 21.42 |
| ATOM | 881 | CA  | TRP | A | 128 | 1.958  | -13.350 | 33.864 | 1.000 | 15.43 |
| ATOM | 882 | CB  | TRP | A | 128 | 1.695  | -14.415 | 34.942 | 1.000 | 17.74 |
| ATOM | 883 | CG  | TRP | A | 128 | 2.565  | -14.200 | 36.157 | 1.000 | 13.35 |

**FIGURE 23**

|      |     |     |     |   |     |        |         |        |       |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 884 | CD1 | TRP | A | 128 | 2.171  | -14.021 | 37.449 | 1.000 | 18.06 |
| ATOM | 885 | NE1 | TRP | A | 128 | 3.264  | -13.857 | 38.263 | 1.000 | 16.29 |
| ATOM | 886 | CE2 | TRP | A | 128 | 4.398  | -13.927 | 37.497 | 1.000 | 13.72 |
| ATOM | 887 | CD2 | TRP | A | 128 | 3.999  | -14.142 | 36.169 | 1.000 | 15.37 |
| ATOM | 888 | CE3 | TRP | A | 128 | 4.986  | -14.251 | 35.178 | 1.000 | 20.85 |
| ATOM | 889 | CZ3 | TRP | A | 128 | 6.319  | -14.148 | 35.521 | 1.000 | 13.01 |
| ATOM | 890 | CH2 | TRP | A | 128 | 6.684  | -13.932 | 36.859 | 1.000 | 20.19 |
| ATOM | 891 | CZ2 | TRP | A | 128 | 5.744  | -13.822 | 37.849 | 1.000 | 22.48 |
| ATOM | 892 | C   | TRP | A | 128 | 1.529  | -13.783 | 32.480 | 1.000 | 11.86 |
| ATOM | 893 | O   | TRP | A | 128 | 2.310  | -14.288 | 31.668 | 1.000 | 21.55 |
| ATOM | 894 | N   | LYS | A | 129 | 0.267  | -13.551 | 32.155 | 1.000 | 16.27 |
| ATOM | 895 | CA  | LYS | A | 129 | -0.214 | -13.821 | 30.798 | 1.000 | 20.73 |
| ATOM | 896 | CB  | LYS | A | 129 | -1.732 | -13.626 | 30.741 | 1.000 | 17.81 |
| ATOM | 897 | CG  | LYS | A | 129 | -2.314 | -13.971 | 29.375 | 1.000 | 25.97 |
| ATOM | 898 | CD  | LYS | A | 129 | -3.752 | -13.477 | 29.289 | 1.000 | 37.98 |
| ATOM | 899 | CE  | LYS | A | 129 | -4.458 | -14.085 | 28.083 | 1.000 | 38.08 |
| ATOM | 900 | NZ  | LYS | A | 129 | -4.700 | -15.547 | 28.280 | 1.000 | 56.47 |
| ATOM | 901 | C   | LYS | A | 129 | 0.480  | -12.919 | 29.785 | 1.000 | 24.29 |
| ATOM | 902 | O   | LYS | A | 129 | 0.862  | -13.346 | 28.692 | 1.000 | 28.21 |
| ATOM | 903 | N   | MET | A | 130 | 0.668  | -11.651 | 30.143 | 1.000 | 19.69 |
| ATOM | 904 | CA  | MET | A | 130 | 1.478  | -10.735 | 29.351 | 1.000 | 15.73 |
| ATOM | 905 | CB  | MET | A | 130 | 1.576  | -9.342  | 29.996 | 1.000 | 13.64 |
| ATOM | 906 | CG  | MET | A | 130 | 2.430  | -8.380  | 29.162 | 1.000 | 18.33 |
| ATOM | 907 | SD  | MET | A | 130 | 2.476  | -6.702  | 29.808 | 1.000 | 23.04 |
| ATOM | 908 | CE  | MET | A | 130 | 3.483  | -6.962  | 31.274 | 1.000 | 22.96 |
| ATOM | 909 | C   | MET | A | 130 | 2.897  | -11.282 | 29.166 | 1.000 | 14.42 |
| ATOM | 910 | O   | MET | A | 130 | 3.384  | -11.324 | 28.034 | 1.000 | 21.88 |
| ATOM | 911 | N   | VAL | A | 131 | 3.537  | -11.664 | 30.266 | 1.000 | 11.85 |
| ATOM | 912 | CA  | VAL | A | 131 | 4.902  | -12.202 | 30.262 | 1.000 | 21.55 |
| ATOM | 913 | CB  | VAL | A | 131 | 5.372  | -12.557 | 31.682 | 1.000 | 18.65 |
| ATOM | 914 | CG1 | VAL | A | 131 | 6.598  | -13.458 | 31.679 | 1.000 | 16.39 |
| ATOM | 915 | CG2 | VAL | A | 131 | 5.688  | -11.303 | 32.508 | 1.000 | 13.87 |
| ATOM | 916 | C   | VAL | A | 131 | 4.984  | -13.418 | 29.333 | 1.000 | 26.29 |
| ATOM | 917 | O   | VAL | A | 131 | 5.892  | -13.533 | 28.500 | 1.000 | 16.82 |
| ATOM | 918 | N   | TRP | A | 132 | 4.026  | -14.334 | 29.437 | 1.000 | 24.10 |
| ATOM | 919 | CA  | TRP | A | 132 | 3.985  | -15.531 | 28.598 | 1.000 | 23.86 |
| ATOM | 920 | CB  | TRP | A | 132 | 2.902  | -16.495 | 29.121 | 1.000 | 27.36 |
| ATOM | 921 | CG  | TRP | A | 132 | 2.771  | -17.754 | 28.310 | 1.000 | 30.80 |
| ATOM | 922 | CD1 | TRP | A | 132 | 1.818  | -18.027 | 27.370 | 1.000 | 36.86 |
| ATOM | 923 | NE1 | TRP | A | 132 | 2.017  | -19.278 | 26.835 | 1.000 | 36.99 |
| ATOM | 924 | CE2 | TRP | A | 132 | 3.115  | -19.844 | 27.424 | 1.000 | 30.56 |
| ATOM | 925 | CD2 | TRP | A | 132 | 3.613  | -18.914 | 28.359 | 1.000 | 24.79 |
| ATOM | 926 | CE3 | TRP | A | 132 | 4.745  | -19.267 | 29.094 | 1.000 | 24.86 |
| ATOM | 927 | CZ3 | TRP | A | 132 | 5.332  | -20.499 | 28.890 | 1.000 | 26.51 |
| ATOM | 928 | CH2 | TRP | A | 132 | 4.813  | -21.405 | 27.955 | 1.000 | 24.87 |
| ATOM | 929 | CZ2 | TRP | A | 132 | 3.706  | -21.089 | 27.215 | 1.000 | 30.31 |
| ATOM | 930 | C   | TRP | A | 132 | 3.747  | -15.207 | 27.129 | 1.000 | 29.34 |
| ATOM | 931 | O   | TRP | A | 132 | 4.450  | -15.695 | 26.237 | 1.000 | 17.82 |
| ATOM | 932 | N   | GLU | A | 133 | 2.744  | -14.379 | 26.835 | 1.000 | 23.54 |
| ATOM | 933 | CA  | GLU | A | 133 | 2.415  | -14.062 | 25.448 | 1.000 | 23.03 |
| ATOM | 934 | CB  | GLU | A | 133 | 1.100  | -13.274 | 25.422 | 1.000 | 27.10 |
| ATOM | 935 | CG  | GLU | A | 133 | -0.095 | -14.176 | 25.718 | 1.000 | 30.65 |

FIGURE 24

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |         |        |       |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 936 | CD  | GLU | A | 133 | -1.396 | -13.399 | 25.736 | 1.000 | 35.26 |
| ATOM | 937 | OE1 | GLU | A | 133 | -1.363 | -12.159 | 25.561 | 1.000 | 34.94 |
| ATOM | 938 | OE2 | GLU | A | 133 | -2.444 | -14.049 | 25.925 | 1.000 | 35.41 |
| ATOM | 939 | C   | GLU | A | 133 | 3.490  | -13.262 | 24.735 | 1.000 | 27.45 |
| ATOM | 940 | O   | GLU | A | 133 | 3.689  | -13.428 | 23.528 | 1.000 | 24.03 |
| ATOM | 941 | N   | GLN | A | 134 | 4.197  | -12.382 | 25.449 | 1.000 | 21.95 |
| ATOM | 942 | CA  | GLN | A | 134 | 5.207  | -11.554 | 24.787 | 1.000 | 17.30 |
| ATOM | 943 | CB  | GLN | A | 134 | 5.310  | -10.184 | 25.466 | 1.000 | 17.87 |
| ATOM | 944 | CG  | GLN | A | 134 | 3.998  | -9.411  | 25.524 | 1.000 | 15.39 |
| ATOM | 945 | CD  | GLN | A | 134 | 3.647  | -8.841  | 24.163 | 1.000 | 19.03 |
| ATOM | 946 | OE1 | GLN | A | 134 | 4.481  | -8.152  | 23.584 | 1.000 | 36.10 |
| ATOM | 947 | NE2 | GLN | A | 134 | 2.453  | -9.133  | 23.668 | 1.000 | 27.56 |
| ATOM | 948 | C   | GLN | A | 134 | 6.576  | -12.214 | 24.782 | 1.000 | 21.51 |
| ATOM | 949 | O   | GLN | A | 134 | 7.556  | -11.579 | 24.396 | 1.000 | 32.24 |
| ATOM | 950 | N   | ASN | A | 135 | 6.677  | -13.476 | 25.207 | 1.000 | 20.76 |
| ATOM | 951 | CA  | ASN | A | 135 | 7.974  | -14.146 | 25.117 | 1.000 | 19.02 |
| ATOM | 952 | CB  | ASN | A | 135 | 8.406  | -14.179 | 23.644 | 1.000 | 24.87 |
| ATOM | 953 | CG  | ASN | A | 135 | 7.566  | -15.129 | 22.810 | 1.000 | 36.12 |
| ATOM | 954 | OD1 | ASN | A | 135 | 7.515  | -16.331 | 23.072 | 1.000 | 34.91 |
| ATOM | 955 | ND2 | ASN | A | 135 | 6.895  | -14.604 | 21.788 | 1.000 | 45.85 |
| ATOM | 956 | C   | ASN | A | 135 | 9.026  | -13.459 | 25.974 | 1.000 | 21.43 |
| ATOM | 957 | O   | ASN | A | 135 | 10.193 | -13.337 | 25.602 | 1.000 | 20.37 |
| ATOM | 958 | N   | VAL | A | 136 | 8.620  | -12.988 | 27.148 | 1.000 | 16.96 |
| ATOM | 959 | CA  | VAL | A | 136 | 9.529  | -12.287 | 28.047 | 1.000 | 15.79 |
| ATOM | 960 | CB  | VAL | A | 136 | 8.719  | -11.486 | 29.093 | 1.000 | 11.80 |
| ATOM | 961 | CG1 | VAL | A | 136 | 9.587  | -11.074 | 30.260 | 1.000 | 9.82  |
| ATOM | 962 | CG2 | VAL | A | 136 | 8.053  | -10.279 | 28.431 | 1.000 | 16.29 |
| ATOM | 963 | C   | VAL | A | 136 | 10.440 | -13.264 | 28.760 | 1.000 | 18.01 |
| ATOM | 964 | O   | VAL | A | 136 | 9.900  | -14.252 | 29.262 | 1.000 | 28.46 |
| ATOM | 965 | N   | HIS | A | 137 | 11.747 | -13.025 | 28.820 | 1.000 | 17.89 |
| ATOM | 966 | CA  | HIS | A | 137 | 12.634 | -13.889 | 29.610 | 1.000 | 21.67 |
| ATOM | 967 | CB  | HIS | A | 137 | 13.724 | -14.513 | 28.743 | 1.000 | 30.48 |
| ATOM | 968 | CG  | HIS | A | 137 | 13.253 | -15.380 | 27.621 | 1.000 | 42.06 |
| ATOM | 969 | ND1 | HIS | A | 137 | 14.124 | -16.077 | 26.808 | 1.000 | 53.39 |
| ATOM | 970 | CE1 | HIS | A | 137 | 13.449 | -16.758 | 25.899 | 1.000 | 51.26 |
| ATOM | 971 | NE2 | HIS | A | 137 | 12.159 | -16.533 | 26.088 | 1.000 | 49.27 |
| ATOM | 972 | CD2 | HIS | A | 137 | 12.018 | -15.676 | 27.154 | 1.000 | 48.02 |
| ATOM | 973 | C   | HIS | A | 137 | 13.263 | -13.116 | 30.766 | 1.000 | 19.36 |
| ATOM | 974 | O   | HIS | A | 137 | 13.818 | -13.683 | 31.703 | 1.000 | 19.33 |
| ATOM | 975 | N   | ASN | A | 138 | 13.190 | -11.780 | 30.748 | 1.000 | 23.51 |
| ATOM | 976 | CA  | ASN | A | 138 | 13.772 | -11.010 | 31.842 | 1.000 | 19.39 |
| ATOM | 977 | CB  | ASN | A | 138 | 15.045 | -10.301 | 31.351 | 1.000 | 21.07 |
| ATOM | 978 | CG  | ASN | A | 138 | 16.123 | -11.316 | 30.999 | 1.000 | 26.12 |
| ATOM | 979 | OD1 | ASN | A | 138 | 16.514 | -11.460 | 29.841 | 1.000 | 27.41 |
| ATOM | 980 | ND2 | ASN | A | 138 | 16.606 | -12.026 | 32.011 | 1.000 | 23.04 |
| ATOM | 981 | C   | ASN | A | 138 | 12.811 | -9.974  | 32.413 | 1.000 | 21.29 |
| ATOM | 982 | O   | ASN | A | 138 | 12.180 | -9.217  | 31.666 | 1.000 | 16.20 |
| ATOM | 983 | N   | ILE | A | 139 | 12.718 | -9.937  | 33.737 | 1.000 | 17.13 |
| ATOM | 984 | CA  | ILE | A | 139 | 11.859 | -8.987  | 34.435 | 1.000 | 16.53 |
| ATOM | 985 | CB  | ILE | A | 139 | 10.693 | -9.655  | 35.187 | 1.000 | 17.07 |
| ATOM | 986 | CG1 | ILE | A | 139 | 9.711  | -10.424 | 34.296 | 1.000 | 17.67 |
| ATOM | 987 | CD1 | ILE | A | 139 | 8.911  | -11.494 | 35.031 | 1.000 | 15.33 |

**FIGURE 25**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 988  | CG2 | ILE | A | 139 | 9.941  | -8.625 | 36.020 | 1.000 | 12.08 |
| ATOM | 989  | C   | ILE | A | 139 | 12.694 | -8.169 | 35.412 | 1.000 | 17.79 |
| ATOM | 990  | O   | ILE | A | 139 | 13.465 | -8.707 | 36.203 | 1.000 | 21.50 |
| ATOM | 991  | N   | VAL | A | 140 | 12.560 | -6.852 | 35.353 | 1.000 | 19.27 |
| ATOM | 992  | CA  | VAL | A | 140 | 13.298 | -5.966 | 36.242 | 1.000 | 20.43 |
| ATOM | 993  | CB  | VAL | A | 140 | 14.088 | -4.892 | 35.469 | 1.000 | 23.29 |
| ATOM | 994  | CG1 | VAL | A | 140 | 14.892 | -4.018 | 36.427 | 1.000 | 15.96 |
| ATOM | 995  | CG2 | VAL | A | 140 | 14.965 | -5.563 | 34.419 | 1.000 | 15.64 |
| ATOM | 996  | C   | VAL | A | 140 | 12.331 | -5.254 | 37.179 | 1.000 | 17.79 |
| ATOM | 997  | O   | VAL | A | 140 | 11.385 | -4.619 | 36.709 | 1.000 | 15.65 |
| ATOM | 998  | N   | MET | A | 141 | 12.596 | -5.376 | 38.473 | 1.000 | 19.78 |
| ATOM | 999  | CA  | MET | A | 141 | 11.718 | -4.726 | 39.452 | 1.000 | 23.36 |
| ATOM | 1000 | CB  | MET | A | 141 | 11.016 | -5.796 | 40.283 | 1.000 | 25.59 |
| ATOM | 1001 | CG  | MET | A | 141 | 10.199 | -5.282 | 41.461 | 1.000 | 21.23 |
| ATOM | 1002 | SD  | MET | A | 141 | 9.408  | -6.648 | 42.325 | 1.000 | 27.56 |
| ATOM | 1003 | CE  | MET | A | 141 | 8.617  | -5.832 | 43.707 | 1.000 | 31.17 |
| ATOM | 1004 | C   | MET | A | 141 | 12.541 | -3.772 | 40.294 | 1.000 | 27.26 |
| ATOM | 1005 | O   | MET | A | 141 | 13.509 | -4.208 | 40.923 | 1.000 | 19.70 |
| ATOM | 1006 | N   | VAL | A | 142 | 12.179 | -2.487 | 40.299 | 1.000 | 22.95 |
| ATOM | 1007 | CA  | VAL | A | 142 | 12.981 | -1.529 | 41.061 | 1.000 | 23.51 |
| ATOM | 1008 | CB  | VAL | A | 142 | 13.642 | -0.457 | 40.171 | 1.000 | 24.01 |
| ATOM | 1009 | CG1 | VAL | A | 142 | 14.774 | -1.104 | 39.384 | 1.000 | 28.07 |
| ATOM | 1010 | CG2 | VAL | A | 142 | 12.631 | 0.200  | 39.250 | 1.000 | 26.62 |
| ATOM | 1011 | C   | VAL | A | 142 | 12.151 | -0.832 | 42.134 | 1.000 | 24.80 |
| ATOM | 1012 | O   | VAL | A | 142 | 12.092 | 0.396  | 42.186 | 1.000 | 24.92 |
| ATOM | 1013 | N   | THR | A | 143 | 11.544 | -1.654 | 42.968 | 1.000 | 32.06 |
| ATOM | 1014 | CA  | THR | A | 143 | 10.713 | -1.262 | 44.092 | 1.000 | 31.60 |
| ATOM | 1015 | CB  | THR | A | 143 | 9.303  | -0.845 | 43.629 | 1.000 | 34.01 |
| ATOM | 1016 | OG1 | THR | A | 143 | 8.553  | -0.296 | 44.720 | 1.000 | 32.56 |
| ATOM | 1017 | CG2 | THR | A | 143 | 8.489  | -2.040 | 43.150 | 1.000 | 19.73 |
| ATOM | 1018 | C   | THR | A | 143 | 10.608 | -2.414 | 45.081 | 1.000 | 32.84 |
| ATOM | 1019 | O   | THR | A | 143 | 10.735 | -3.579 | 44.697 | 1.000 | 27.98 |
| ATOM | 1020 | N   | GLN | A | 144 | 10.371 | -2.074 | 46.348 | 1.000 | 33.83 |
| ATOM | 1021 | CA  | GLN | A | 144 | 9.992  | -3.090 | 47.327 | 1.000 | 31.46 |
| ATOM | 1022 | CB  | GLN | A | 144 | 10.464 | -2.772 | 48.733 | 1.000 | 28.66 |
| ATOM | 1023 | CG  | GLN | A | 144 | 11.964 | -2.806 | 48.954 | 1.000 | 39.24 |
| ATOM | 1024 | CD  | GLN | A | 144 | 12.357 | -2.317 | 50.339 | 1.000 | 47.09 |
| ATOM | 1025 | OE1 | GLN | A | 144 | 12.240 | -3.049 | 51.324 | 1.000 | 40.08 |
| ATOM | 1026 | NE2 | GLN | A | 144 | 12.828 | -1.075 | 50.438 | 1.000 | 32.97 |
| ATOM | 1027 | C   | GLN | A | 144 | 8.469  | -3.184 | 47.268 | 1.000 | 30.87 |
| ATOM | 1028 | O   | GLN | A | 144 | 7.859  | -2.272 | 46.701 | 1.000 | 27.64 |
| ATOM | 1029 | N   | CYS | A | 145 | 7.887  | -4.240 | 47.815 | 1.000 | 32.97 |
| ATOM | 1030 | CA  | CYS | A | 145 | 6.434  | -4.376 | 47.762 | 1.000 | 27.50 |
| ATOM | 1031 | CB  | CYS | A | 145 | 6.053  | -5.820 | 48.082 | 1.000 | 24.78 |
| ATOM | 1032 | SG  | CYS | A | 145 | 6.485  | -6.965 | 46.749 | 1.000 | 32.93 |
| ATOM | 1033 | C   | CYS | A | 145 | 5.746  | -3.404 | 48.716 | 1.000 | 29.39 |
| ATOM | 1034 | O   | CYS | A | 145 | 4.579  | -3.052 | 48.520 | 1.000 | 29.75 |
| ATOM | 1035 | N   | VAL | A | 146 | 6.480  | -2.988 | 49.733 | 1.000 | 32.17 |
| ATOM | 1036 | CA  | VAL | A | 146 | 6.060  | -2.022 | 50.744 | 1.000 | 32.69 |
| ATOM | 1037 | CB  | VAL | A | 146 | 5.547  | -2.672 | 52.039 | 1.000 | 35.63 |
| ATOM | 1038 | CG1 | VAL | A | 146 | 4.981  | -1.619 | 52.989 | 1.000 | 28.22 |
| ATOM | 1039 | CG2 | VAL | A | 146 | 4.490  | -3.724 | 51.746 | 1.000 | 39.32 |

**FIGURE 26**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1040 | C   | VAL | A | 146 | 7.238  | -1.119 | 51.101 | 1.000 | 24.56 |
| ATOM | 1041 | O   | VAL | A | 146 | 8.312  | -1.600 | 51.466 | 1.000 | 30.54 |
| ATOM | 1042 | N   | GLU | A | 147 | 7.053  | 0.184  | 50.987 | 1.000 | 26.82 |
| ATOM | 1043 | CA  | GLU | A | 147 | 8.128  | 1.123  | 51.322 | 1.000 | 34.58 |
| ATOM | 1044 | CB  | GLU | A | 147 | 8.516  | 1.929  | 50.080 | 1.000 | 36.31 |
| ATOM | 1045 | CG  | GLU | A | 147 | 8.591  | 1.048  | 48.834 | 1.000 | 43.83 |
| ATOM | 1046 | CD  | GLU | A | 147 | 9.589  | 1.535  | 47.809 | 1.000 | 42.03 |
| ATOM | 1047 | OE1 | GLU | A | 147 | 9.517  | 2.715  | 47.414 | 1.000 | 36.27 |
| ATOM | 1048 | OE2 | GLU | A | 147 | 10.460 | 0.748  | 47.383 | 1.000 | 38.56 |
| ATOM | 1049 | C   | GLU | A | 147 | 7.682  | 2.020  | 52.466 | 1.000 | 43.00 |
| ATOM | 1050 | O   | GLU | A | 147 | 6.842  | 2.895  | 52.262 | 1.000 | 36.39 |
| ATOM | 1051 | N   | LYS | A | 148 | 8.228  | 1.770  | 53.651 | 1.000 | 53.50 |
| ATOM | 1052 | CA  | LYS | A | 148 | 7.803  | 2.440  | 54.874 | 1.000 | 50.57 |
| ATOM | 1053 | CB  | LYS | A | 148 | 8.242  | 3.904  | 54.859 | 1.000 | 53.82 |
| ATOM | 1054 | CG  | LYS | A | 148 | 9.487  | 4.175  | 55.693 | 1.000 | 55.76 |
| ATOM | 1055 | CD  | LYS | A | 148 | 9.736  | 5.666  | 55.836 | 1.000 | 61.51 |
| ATOM | 1056 | CE  | LYS | A | 148 | 11.217 | 5.994  | 55.917 | 1.000 | 64.59 |
| ATOM | 1057 | NZ  | LYS | A | 148 | 11.582 | 7.165  | 55.066 | 1.000 | 54.71 |
| ATOM | 1058 | C   | LYS | A | 148 | 6.291  | 2.327  | 55.068 | 1.000 | 40.10 |
| ATOM | 1059 | O   | LYS | A | 148 | 5.588  | 3.337  | 55.119 | 1.000 | 40.70 |
| ATOM | 1060 | N   | GLY | A | 149 | 5.792  | 1.102  | 55.161 | 1.000 | 31.76 |
| ATOM | 1061 | CA  | GLY | A | 149 | 4.396  | 0.812  | 55.408 | 1.000 | 38.69 |
| ATOM | 1062 | C   | GLY | A | 149 | 3.455  | 1.021  | 54.249 | 1.000 | 45.94 |
| ATOM | 1063 | O   | GLY | A | 149 | 2.303  | 0.575  | 54.255 | 1.000 | 42.79 |
| ATOM | 1064 | N   | ARG | A | 150 | 3.889  | 1.707  | 53.188 | 1.000 | 44.38 |
| ATOM | 1065 | CA  | ARG | A | 150 | 2.967  | 1.932  | 52.076 | 1.000 | 37.05 |
| ATOM | 1066 | CB  | ARG | A | 150 | 3.179  | 3.306  | 51.450 | 1.000 | 43.59 |
| ATOM | 1067 | CG  | ARG | A | 150 | 2.273  | 4.410  | 51.971 | 1.000 | 52.87 |
| ATOM | 1068 | CD  | ARG | A | 150 | 2.530  | 5.696  | 51.196 | 1.000 | 65.25 |
| ATOM | 1069 | NE  | ARG | A | 150 | 1.626  | 6.786  | 51.559 | 1.000 | 75.91 |
| ATOM | 1070 | CZ  | ARG | A | 150 | 1.738  | 8.024  | 51.087 | 1.000 | 82.71 |
| ATOM | 1071 | NH1 | ARG | A | 150 | 2.708  | 8.322  | 50.240 | 1.000 | 99.14 |
| ATOM | 1072 | NH2 | ARG | A | 150 | 0.886  | 8.969  | 51.456 | 1.000 | 75.70 |
| ATOM | 1073 | C   | ARG | A | 150 | 3.144  | 0.849  | 51.015 | 1.000 | 31.26 |
| ATOM | 1074 | O   | ARG | A | 150 | 4.266  | 0.643  | 50.541 | 1.000 | 26.56 |
| ATOM | 1075 | N   | VAL | A | 151 | 2.039  | 0.197  | 50.671 | 1.000 | 26.68 |
| ATOM | 1076 | CA  | VAL | A | 151 | 2.035  | -0.861 | 49.673 | 1.000 | 27.32 |
| ATOM | 1077 | CB  | VAL | A | 151 | 0.713  | -1.647 | 49.660 | 1.000 | 35.52 |
| ATOM | 1078 | CG1 | VAL | A | 151 | 0.755  | -2.776 | 48.637 | 1.000 | 33.72 |
| ATOM | 1079 | CG2 | VAL | A | 151 | 0.441  | -2.202 | 51.049 | 1.000 | 18.61 |
| ATOM | 1080 | C   | VAL | A | 151 | 2.298  | -0.281 | 48.288 | 1.000 | 28.80 |
| ATOM | 1081 | O   | VAL | A | 151 | 1.563  | 0.579  | 47.806 | 1.000 | 38.64 |
| ATOM | 1082 | N   | LYS | A | 152 | 3.371  | -0.759 | 47.674 | 1.000 | 33.79 |
| ATOM | 1083 | CA  | LYS | A | 152 | 3.788  | -0.282 | 46.358 | 1.000 | 32.44 |
| ATOM | 1084 | CB  | LYS | A | 152 | 5.272  | 0.088  | 46.373 | 1.000 | 29.41 |
| ATOM | 1085 | CG  | LYS | A | 152 | 5.626  | 1.158  | 47.393 | 1.000 | 38.23 |
| ATOM | 1086 | CD  | LYS | A | 152 | 4.469  | 2.111  | 47.631 | 1.000 | 43.28 |
| ATOM | 1087 | CE  | LYS | A | 152 | 4.900  | 3.566  | 47.538 | 1.000 | 49.33 |
| ATOM | 1088 | NZ  | LYS | A | 152 | 3.834  | 4.403  | 46.910 | 1.000 | 76.06 |
| ATOM | 1089 | C   | LYS | A | 152 | 3.528  | -1.344 | 45.298 | 1.000 | 30.77 |
| ATOM | 1090 | O   | LYS | A | 152 | 3.227  | -1.024 | 44.149 | 1.000 | 33.84 |
| ATOM | 1091 | N   | CYS | A | 153 | 3.648  | -2.611 | 45.697 | 1.000 | 27.03 |

**FIGURE 27**

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1092 | CA  | CYS | A | 153 | 3.476  | -3.698  | 44.729 | 1.000 | 27.81 |
| ATOM | 1093 | CB  | CYS | A | 153 | 4.776  | -3.878  | 43.946 | 1.000 | 27.07 |
| ATOM | 1094 | SG  | CYS | A | 153 | 4.790  | -5.091  | 42.611 | 1.000 | 26.17 |
| ATOM | 1095 | C   | CYS | A | 153 | 3.064  | -4.986  | 45.420 | 1.000 | 26.82 |
| ATOM | 1096 | O   | CYS | A | 153 | 3.553  | -5.324  | 46.490 | 1.000 | 27.44 |
| ATOM | 1097 | N   | ASP | A | 154 | 2.155  | -5.742  | 44.804 | 1.000 | 34.85 |
| ATOM | 1098 | CA  | ASP | A | 154 | 1.828  | -7.062  | 45.322 | 1.000 | 37.76 |
| ATOM | 1099 | CB  | ASP | A | 154 | 0.584  | -7.638  | 44.645 | 1.000 | 29.89 |
| ATOM | 1100 | CG  | ASP | A | 154 | 0.099  | -8.911  | 45.316 | 1.000 | 34.93 |
| ATOM | 1101 | OD1 | ASP | A | 154 | -0.148 | -9.919  | 44.627 | 1.000 | 38.18 |
| ATOM | 1102 | OD2 | ASP | A | 154 | -0.042 | -8.917  | 46.557 | 1.000 | 47.22 |
| ATOM | 1103 | C   | ASP | A | 154 | 3.010  | -8.017  | 45.130 | 1.000 | 40.61 |
| ATOM | 1104 | O   | ASP | A | 154 | 3.825  | -7.877  | 44.216 | 1.000 | 30.25 |
| ATOM | 1105 | N   | HIS | A | 155 | 3.097  | -8.993  | 46.020 | 1.000 | 32.47 |
| ATOM | 1106 | CA  | HIS | A | 155 | 4.072  | -10.070 | 45.914 | 1.000 | 30.20 |
| ATOM | 1107 | CB  | HIS | A | 155 | 4.312  | -10.721 | 47.282 | 1.000 | 28.22 |
| ATOM | 1108 | CG  | HIS | A | 155 | 5.365  | -11.788 | 47.244 | 1.000 | 30.06 |
| ATOM | 1109 | ND1 | HIS | A | 155 | 6.655  | -11.595 | 47.686 | 1.000 | 32.04 |
| ATOM | 1110 | CE1 | HIS | A | 155 | 7.357  | -12.700 | 47.514 | 1.000 | 31.07 |
| ATOM | 1111 | NE2 | HIS | A | 155 | 6.557  | -13.606 | 46.980 | 1.000 | 35.21 |
| ATOM | 1112 | CD2 | HIS | A | 155 | 5.311  | -13.064 | 46.793 | 1.000 | 27.75 |
| ATOM | 1113 | C   | HIS | A | 155 | 3.531  | -11.053 | 44.879 | 1.000 | 30.27 |
| ATOM | 1114 | O   | HIS | A | 155 | 2.745  | -11.922 | 45.253 | 1.000 | 34.64 |
| ATOM | 1115 | N   | TYR | A | 156 | 3.914  | -10.897 | 43.613 | 1.000 | 24.90 |
| ATOM | 1116 | CA  | TYR | A | 156 | 3.234  | -11.590 | 42.521 | 1.000 | 22.68 |
| ATOM | 1117 | CB  | TYR | A | 156 | 3.093  | -10.621 | 41.340 | 1.000 | 22.68 |
| ATOM | 1118 | CG  | TYR | A | 156 | 4.387  | -10.046 | 40.818 | 1.000 | 21.15 |
| ATOM | 1119 | CD1 | TYR | A | 156 | 5.101  | -10.741 | 39.844 | 1.000 | 20.48 |
| ATOM | 1120 | CE1 | TYR | A | 156 | 6.286  | -10.236 | 39.348 | 1.000 | 18.15 |
| ATOM | 1121 | CZ  | TYR | A | 156 | 6.755  | -9.037  | 39.824 | 1.000 | 18.02 |
| ATOM | 1122 | OH  | TYR | A | 156 | 7.933  | -8.545  | 39.322 | 1.000 | 19.23 |
| ATOM | 1123 | CE2 | TYR | A | 156 | 6.070  | -8.320  | 40.786 | 1.000 | 19.56 |
| ATOM | 1124 | CD2 | TYR | A | 156 | 4.883  | -8.836  | 41.274 | 1.000 | 17.13 |
| ATOM | 1125 | C   | TYR | A | 156 | 3.905  | -12.870 | 42.063 | 1.000 | 25.52 |
| ATOM | 1126 | O   | TYR | A | 156 | 3.550  | -13.447 | 41.027 | 1.000 | 22.83 |
| ATOM | 1127 | N   | TRP | A | 157 | 4.881  | -13.356 | 42.825 | 1.000 | 33.11 |
| ATOM | 1128 | CA  | TRP | A | 157 | 5.531  | -14.623 | 42.504 | 1.000 | 31.82 |
| ATOM | 1129 | CB  | TRP | A | 157 | 6.985  | -14.383 | 42.092 | 1.000 | 32.50 |
| ATOM | 1130 | CG  | TRP | A | 157 | 7.827  | -13.805 | 43.197 | 1.000 | 31.35 |
| ATOM | 1131 | CD1 | TRP | A | 157 | 8.582  | -14.486 | 44.110 | 1.000 | 27.90 |
| ATOM | 1132 | NE1 | TRP | A | 157 | 9.208  | -13.611 | 44.960 | 1.000 | 24.08 |
| ATOM | 1133 | CE2 | TRP | A | 157 | 8.866  | -12.330 | 44.607 | 1.000 | 25.03 |
| ATOM | 1134 | CD2 | TRP | A | 157 | 8.000  | -12.414 | 43.503 | 1.000 | 28.13 |
| ATOM | 1135 | CE3 | TRP | A | 157 | 7.500  | -11.231 | 42.944 | 1.000 | 23.89 |
| ATOM | 1136 | CZ3 | TRP | A | 157 | 7.880  | -10.030 | 43.502 | 1.000 | 22.95 |
| ATOM | 1137 | CH2 | TRP | A | 157 | 8.743  | -9.975  | 44.602 | 1.000 | 25.46 |
| ATOM | 1138 | CZ2 | TRP | A | 157 | 9.251  | -11.113 | 45.172 | 1.000 | 27.53 |
| ATOM | 1139 | C   | TRP | A | 157 | 5.490  | -15.556 | 43.706 | 1.000 | 28.64 |
| ATOM | 1140 | O   | TRP | A | 157 | 5.361  | -15.056 | 44.828 | 1.000 | 33.96 |
| ATOM | 1141 | N   | PRO | A | 158 | 5.623  | -16.858 | 43.503 | 1.000 | 30.31 |
| ATOM | 1142 | CA  | PRO | A | 158 | 5.666  | -17.787 | 44.640 | 1.000 | 33.91 |
| ATOM | 1143 | CB  | PRO | A | 158 | 5.597  | -19.170 | 44.009 | 1.000 | 24.17 |

**FIGURE 28**



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1144 | CG  | PRO | A | 158 | 5.988  | -18.987 | 42.583 | 1.000 | 30.62 |
| ATOM | 1145 | CD  | PRO | A | 158 | 5.757  | -17.553 | 42.215 | 1.000 | 28.57 |
| ATOM | 1146 | C   | PRO | A | 158 | 6.990  | -17.602 | 45.391 | 1.000 | 42.64 |
| ATOM | 1147 | O   | PRO | A | 158 | 8.051  | -17.797 | 44.790 | 1.000 | 41.28 |
| ATOM | 1148 | N   | ALA | A | 159 | 6.903  | -17.227 | 46.657 | 1.000 | 44.31 |
| ATOM | 1149 | CA  | ALA | A | 159 | 8.044  | -16.897 | 47.500 | 1.000 | 52.40 |
| ATOM | 1150 | CB  | ALA | A | 159 | 7.567  | -16.083 | 48.701 | 1.000 | 39.50 |
| ATOM | 1151 | C   | ALA | A | 159 | 8.838  | -18.094 | 48.000 | 1.000 | 52.74 |
| ATOM | 1152 | O   | ALA | A | 159 | 9.922  | -17.935 | 48.572 | 1.000 | 69.24 |
| ATOM | 1153 | N   | ASP | A | 160 | 8.338  | -19.307 | 47.809 | 1.000 | 51.47 |
| ATOM | 1154 | CA  | ASP | A | 160 | 9.110  | -20.487 | 48.190 | 1.000 | 60.84 |
| ATOM | 1155 | CB  | ASP | A | 160 | 8.266  | -21.507 | 48.945 | 1.000 | 68.39 |
| ATOM | 1156 | CG  | ASP | A | 160 | 7.989  | -21.175 | 50.394 | 1.000 | 75.02 |
| ATOM | 1157 | OD1 | ASP | A | 160 | 8.838  | -20.519 | 51.035 | 1.000 | 88.56 |
| ATOM | 1158 | OD2 | ASP | A | 160 | 6.913  | -21.574 | 50.891 | 1.000 | 76.88 |
| ATOM | 1159 | C   | ASP | A | 160 | 9.663  | -21.134 | 46.924 | 1.000 | 53.11 |
| ATOM | 1160 | O   | ASP | A | 160 | 9.452  | -20.618 | 45.827 | 1.000 | 52.42 |
| ATOM | 1161 | N   | GLN | A | 161 | 10.327 | -22.273 | 47.064 | 1.000 | 49.61 |
| ATOM | 1162 | CA  | GLN | A | 161 | 10.738 | -23.062 | 45.911 | 1.000 | 54.59 |
| ATOM | 1163 | CB  | GLN | A | 161 | 11.818 | -24.073 | 46.306 | 1.000 | 56.30 |
| ATOM | 1164 | CG  | GLN | A | 161 | 13.239 | -23.547 | 46.201 | 1.000 | 55.95 |
| ATOM | 1165 | CD  | GLN | A | 161 | 13.450 | -22.701 | 44.959 | 1.000 | 53.24 |
| ATOM | 1166 | OE1 | GLN | A | 161 | 13.368 | -23.208 | 43.842 | 1.000 | 49.06 |
| ATOM | 1167 | NE2 | GLN | A | 161 | 13.724 | -21.415 | 45.153 | 1.000 | 41.80 |
| ATOM | 1168 | C   | GLN | A | 161 | 9.543  | -23.794 | 45.301 | 1.000 | 51.44 |
| ATOM | 1169 | O   | GLN | A | 161 | 9.666  | -24.493 | 44.295 | 1.000 | 52.78 |
| ATOM | 1170 | N   | ASP | A | 162 | 8.381  | -23.641 | 45.922 | 1.000 | 45.89 |
| ATOM | 1171 | CA  | ASP | A | 162 | 7.149  | -24.258 | 45.482 | 1.000 | 51.10 |
| ATOM | 1172 | CB  | ASP | A | 162 | 6.101  | -24.204 | 46.603 | 1.000 | 57.35 |
| ATOM | 1173 | CG  | ASP | A | 162 | 5.884  | -22.779 | 47.078 | 1.000 | 65.40 |
| ATOM | 1174 | OD1 | ASP | A | 162 | 6.698  | -21.916 | 46.685 | 1.000 | 69.28 |
| ATOM | 1175 | OD2 | ASP | A | 162 | 4.914  | -22.539 | 47.823 | 1.000 | 75.26 |
| ATOM | 1176 | C   | ASP | A | 162 | 6.603  | -23.596 | 44.219 | 1.000 | 49.85 |
| ATOM | 1177 | O   | ASP | A | 162 | 7.291  | -22.878 | 43.496 | 1.000 | 53.02 |
| ATOM | 1178 | N   | SER | A | 163 | 5.331  | -23.884 | 43.972 | 1.000 | 41.47 |
| ATOM | 1179 | CA  | SER | A | 163 | 4.634  | -23.472 | 42.768 | 1.000 | 32.87 |
| ATOM | 1180 | CB  | SER | A | 163 | 4.486  | -24.685 | 41.840 | 1.000 | 32.47 |
| ATOM | 1181 | OG  | SER | A | 163 | 3.800  | -25.721 | 42.529 | 1.000 | 31.33 |
| ATOM | 1182 | C   | SER | A | 163 | 3.257  | -22.894 | 43.072 | 1.000 | 32.86 |
| ATOM | 1183 | O   | SER | A | 163 | 2.679  | -23.132 | 44.135 | 1.000 | 30.48 |
| ATOM | 1184 | N   | LEU | A | 164 | 2.739  | -22.138 | 42.115 | 1.000 | 28.27 |
| ATOM | 1185 | CA  | LEU | A | 164 | 1.390  | -21.603 | 42.172 | 1.000 | 23.14 |
| ATOM | 1186 | CB  | LEU | A | 164 | 1.320  | -20.222 | 42.813 | 1.000 | 23.52 |
| ATOM | 1187 | CG  | LEU | A | 164 | 1.908  | -20.041 | 44.206 | 1.000 | 37.76 |
| ATOM | 1188 | CD1 | LEU | A | 164 | 1.918  | -18.560 | 44.569 | 1.000 | 36.50 |
| ATOM | 1189 | CD2 | LEU | A | 164 | 1.141  | -20.859 | 45.236 | 1.000 | 38.57 |
| ATOM | 1190 | C   | LEU | A | 164 | 0.833  | -21.459 | 40.757 | 1.000 | 28.03 |
| ATOM | 1191 | O   | LEU | A | 164 | 1.613  | -21.308 | 39.816 | 1.000 | 24.57 |
| ATOM | 1192 | N   | TYR | A | 165 | -0.492 | -21.480 | 40.677 | 1.000 | 28.64 |
| ATOM | 1193 | CA  | TYR | A | 165 | -1.157 | -21.136 | 39.432 | 1.000 | 28.93 |
| ATOM | 1194 | CB  | TYR | A | 165 | -2.517 | -21.817 | 39.316 | 1.000 | 22.72 |
| ATOM | 1195 | CG  | TYR | A | 165 | -2.482 | -23.276 | 38.942 | 1.000 | 18.62 |

**FIGURE 29**

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1196 | CD1 | TYR | A | 165 | -2.328 | -24.260 | 39.911 | 1.000 | 25.83 |
| ATOM | 1197 | CE1 | TYR | A | 165 | -2.294 | -25.603 | 39.581 | 1.000 | 25.94 |
| ATOM | 1198 | CZ  | TYR | A | 165 | -2.418 | -25.987 | 38.262 | 1.000 | 26.30 |
| ATOM | 1199 | OH  | TYR | A | 165 | -2.393 | -27.324 | 37.926 | 1.000 | 27.99 |
| ATOM | 1200 | CE2 | TYR | A | 165 | -2.577 | -25.035 | 37.287 | 1.000 | 21.27 |
| ATOM | 1201 | CD2 | TYR | A | 165 | -2.606 | -23.693 | 37.627 | 1.000 | 22.96 |
| ATOM | 1202 | C   | TYR | A | 165 | -1.349 | -19.620 | 39.364 | 1.000 | 30.51 |
| ATOM | 1203 | O   | TYR | A | 165 | -1.633 | -19.005 | 40.383 | 1.000 | 27.58 |
| ATOM | 1204 | N   | TYR | A | 166 | -1.205 | -19.047 | 38.185 | 1.000 | 24.74 |
| ATOM | 1205 | CA  | TYR | A | 166 | -1.612 | -17.675 | 37.914 | 1.000 | 24.22 |
| ATOM | 1206 | CB  | TYR | A | 166 | -0.422 | -16.731 | 37.786 | 1.000 | 24.27 |
| ATOM | 1207 | CG  | TYR | A | 166 | 0.394  | -16.584 | 39.057 | 1.000 | 25.75 |
| ATOM | 1208 | CD1 | TYR | A | 166 | 0.075  | -15.624 | 40.015 | 1.000 | 21.51 |
| ATOM | 1209 | CE1 | TYR | A | 166 | 0.820  | -15.483 | 41.177 | 1.000 | 23.56 |
| ATOM | 1210 | CZ  | TYR | A | 166 | 1.899  | -16.316 | 41.394 | 1.000 | 24.64 |
| ATOM | 1211 | OH  | TYR | A | 166 | 2.646  | -16.197 | 42.543 | 1.000 | 25.20 |
| ATOM | 1212 | CE2 | TYR | A | 166 | 2.244  | -17.280 | 40.464 | 1.000 | 21.31 |
| ATOM | 1213 | CD2 | TYR | A | 166 | 1.492  | -17.401 | 39.306 | 1.000 | 28.88 |
| ATOM | 1214 | C   | TYR | A | 166 | -2.449 | -17.749 | 36.642 | 1.000 | 28.89 |
| ATOM | 1215 | O   | TYR | A | 166 | -1.923 | -17.886 | 35.535 | 1.000 | 28.35 |
| ATOM | 1216 | N   | GLY | A | 167 | -3.775 | -17.705 | 36.793 | 1.000 | 30.71 |
| ATOM | 1217 | CA  | GLY | A | 167 | -4.586 | -17.861 | 35.583 | 1.000 | 35.47 |
| ATOM | 1218 | C   | GLY | A | 167 | -4.383 | -19.271 | 35.038 | 1.000 | 34.48 |
| ATOM | 1219 | O   | GLY | A | 167 | -4.521 | -20.213 | 35.826 | 1.000 | 29.66 |
| ATOM | 1220 | N   | ASP | A | 168 | -4.072 | -19.391 | 33.760 | 1.000 | 25.86 |
| ATOM | 1221 | CA  | ASP | A | 168 | -3.860 | -20.665 | 33.082 | 1.000 | 23.07 |
| ATOM | 1222 | CB  | ASP | A | 168 | -4.216 | -20.560 | 31.601 | 1.000 | 22.17 |
| ATOM | 1223 | CG  | ASP | A | 168 | -5.719 | -20.526 | 31.403 | 1.000 | 30.38 |
| ATOM | 1224 | OD1 | ASP | A | 168 | -6.422 | -20.536 | 32.432 | 1.000 | 44.55 |
| ATOM | 1225 | OD2 | ASP | A | 168 | -6.178 | -20.501 | 30.246 | 1.000 | 52.57 |
| ATOM | 1226 | C   | ASP | A | 168 | -2.411 | -21.110 | 33.207 | 1.000 | 28.96 |
| ATOM | 1227 | O   | ASP | A | 168 | -1.997 | -22.187 | 32.785 | 1.000 | 35.10 |
| ATOM | 1228 | N   | LEU | A | 169 | -1.617 | -20.229 | 33.816 | 1.000 | 33.00 |
| ATOM | 1229 | CA  | LEU | A | 169 | -0.197 | -20.558 | 33.927 | 1.000 | 32.77 |
| ATOM | 1230 | CB  | LEU | A | 169 | 0.652  | -19.326 | 33.571 | 1.000 | 25.71 |
| ATOM | 1231 | CG  | LEU | A | 169 | 0.116  | -18.558 | 32.353 | 1.000 | 24.37 |
| ATOM | 1232 | CD1 | LEU | A | 169 | 0.491  | -17.088 | 32.434 | 1.000 | 31.21 |
| ATOM | 1233 | CD2 | LEU | A | 169 | 0.634  | -19.191 | 31.076 | 1.000 | 35.13 |
| ATOM | 1234 | C   | LEU | A | 169 | 0.190  | -21.063 | 35.306 | 1.000 | 20.10 |
| ATOM | 1235 | O   | LEU | A | 169 | -0.332 | -20.698 | 36.352 | 1.000 | 25.85 |
| ATOM | 1236 | N   | ILE | A | 170 | 1.186  | -21.938 | 35.253 | 1.000 | 23.95 |
| ATOM | 1237 | CA  | ILE | A | 170 | 1.792  | -22.432 | 36.482 | 1.000 | 30.46 |
| ATOM | 1238 | CB  | ILE | A | 170 | 1.748  | -23.965 | 36.556 | 1.000 | 29.06 |
| ATOM | 1239 | CG1 | ILE | A | 170 | 2.820  | -24.536 | 37.485 | 1.000 | 31.61 |
| ATOM | 1240 | CD1 | ILE | A | 170 | 2.381  | -24.474 | 38.935 | 1.000 | 36.97 |
| ATOM | 1241 | CG2 | ILE | A | 170 | 1.824  | -24.585 | 35.175 | 1.000 | 61.97 |
| ATOM | 1242 | C   | ILE | A | 170 | 3.229  | -21.924 | 36.541 | 1.000 | 27.52 |
| ATOM | 1243 | O   | ILE | A | 170 | 3.980  | -22.051 | 35.579 | 1.000 | 28.50 |
| ATOM | 1244 | N   | LEU | A | 171 | 3.581  | -21.324 | 37.663 | 1.000 | 33.56 |
| ATOM | 1245 | CA  | LEU | A | 171 | 4.899  | -20.758 | 37.889 | 1.000 | 23.37 |
| ATOM | 1246 | CB  | LEU | A | 171 | 4.752  | -19.251 | 38.120 | 1.000 | 35.18 |
| ATOM | 1247 | CG  | LEU | A | 171 | 5.997  | -18.414 | 37.823 | 1.000 | 43.60 |

**FIGURE 30**

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1248 | CD1 | LEU | A | 171 | 5.642  | -17.121 | 37.111 | 1.000 | 63.91 |
| ATOM | 1249 | CD2 | LEU | A | 171 | 6.736  | -18.133 | 39.121 | 1.000 | 45.12 |
| ATOM | 1250 | C   | LEU | A | 171 | 5.591  | -21.435 | 39.061 | 1.000 | 27.57 |
| ATOM | 1251 | O   | LEU | A | 171 | 5.001  | -21.717 | 40.109 | 1.000 | 26.54 |
| ATOM | 1252 | N   | GLN | A | 172 | 6.879  | -21.712 | 38.886 | 1.000 | 33.32 |
| ATOM | 1253 | CA  | GLN | A | 172 | 7.659  | -22.398 | 39.914 | 1.000 | 32.37 |
| ATOM | 1254 | CB  | GLN | A | 172 | 7.941  | -23.825 | 39.432 | 1.000 | 29.07 |
| ATOM | 1255 | CG  | GLN | A | 172 | 8.747  | -24.687 | 40.384 | 1.000 | 30.68 |
| ATOM | 1256 | CD  | GLN | A | 172 | 9.108  | -26.026 | 39.763 | 1.000 | 33.95 |
| ATOM | 1257 | OE1 | GLN | A | 172 | 9.084  | -26.176 | 38.543 | 1.000 | 34.24 |
| ATOM | 1258 | NE2 | GLN | A | 172 | 9.436  | -27.007 | 40.589 | 1.000 | 42.96 |
| ATOM | 1259 | C   | GLN | A | 172 | 8.953  | -21.663 | 40.192 | 1.000 | 26.84 |
| ATOM | 1260 | O   | GLN | A | 172 | 9.698  | -21.353 | 39.268 | 1.000 | 27.43 |
| ATOM | 1261 | N   | MET | A | 173 | 9.304  | -21.339 | 41.437 | 1.000 | 32.50 |
| ATOM | 1262 | CA  | MET | A | 173 | 10.597 | -20.678 | 41.595 | 1.000 | 30.97 |
| ATOM | 1263 | CB  | MET | A | 173 | 10.693 | -19.860 | 42.883 | 1.000 | 29.94 |
| ATOM | 1264 | CG  | MET | A | 173 | 12.132 | -19.396 | 43.134 | 1.000 | 34.61 |
| ATOM | 1265 | SD  | MET | A | 173 | 12.197 | -18.091 | 44.380 | 1.000 | 57.02 |
| ATOM | 1266 | CE  | MET | A | 173 | 12.001 | -19.065 | 45.860 | 1.000 | 24.26 |
| ATOM | 1267 | C   | MET | A | 173 | 11.719 | -21.715 | 41.612 | 1.000 | 36.84 |
| ATOM | 1268 | O   | MET | A | 173 | 11.649 | -22.640 | 42.427 | 1.000 | 50.73 |
| ATOM | 1269 | N   | LEU | A | 174 | 12.703 | -21.541 | 40.741 | 1.000 | 29.04 |
| ATOM | 1270 | CA  | LEU | A | 174 | 13.805 | -22.491 | 40.663 | 1.000 | 33.35 |
| ATOM | 1271 | CB  | LEU | A | 174 | 14.272 | -22.638 | 39.215 | 1.000 | 28.88 |
| ATOM | 1272 | CG  | LEU | A | 174 | 13.322 | -23.341 | 38.253 | 1.000 | 37.78 |
| ATOM | 1273 | CD1 | LEU | A | 174 | 13.953 | -23.473 | 36.869 | 1.000 | 27.40 |
| ATOM | 1274 | CD2 | LEU | A | 174 | 12.907 | -24.710 | 38.769 | 1.000 | 40.70 |
| ATOM | 1275 | C   | LEU | A | 174 | 14.990 | -22.089 | 41.532 | 1.000 | 40.05 |
| ATOM | 1276 | O   | LEU | A | 174 | 15.816 | -22.939 | 41.869 | 1.000 | 47.76 |
| ATOM | 1277 | N   | SER | A | 175 | 15.096 | -20.812 | 41.884 | 1.000 | 40.28 |
| ATOM | 1278 | CA  | SER | A | 175 | 16.267 | -20.331 | 42.611 | 1.000 | 36.37 |
| ATOM | 1279 | CB  | SER | A | 175 | 17.521 | -20.496 | 41.750 | 1.000 | 41.94 |
| ATOM | 1280 | OG  | SER | A | 175 | 17.651 | -19.439 | 40.814 | 1.000 | 42.50 |
| ATOM | 1281 | C   | SER | A | 175 | 16.120 | -18.877 | 43.028 | 1.000 | 33.27 |
| ATOM | 1282 | O   | SER | A | 175 | 15.231 | -18.146 | 42.597 | 1.000 | 31.30 |
| ATOM | 1283 | N   | GLU | A | 176 | 17.016 | -18.426 | 43.908 | 1.000 | 21.04 |
| ATOM | 1284 | CA  | GLU | A | 176 | 16.840 | -17.086 | 44.444 | 1.000 | 28.91 |
| ATOM | 1285 | CB  | GLU | A | 176 | 15.621 | -17.013 | 45.373 | 1.000 | 31.33 |
| ATOM | 1286 | CG  | GLU | A | 176 | 15.576 | -15.684 | 46.108 | 1.000 | 33.37 |
| ATOM | 1287 | CD  | GLU | A | 176 | 14.525 | -15.568 | 47.187 | 1.000 | 40.95 |
| ATOM | 1288 | OE1 | GLU | A | 176 | 14.831 | -15.906 | 48.350 | 1.000 | 66.50 |
| ATOM | 1289 | OE2 | GLU | A | 176 | 13.390 | -15.121 | 46.900 | 1.000 | 42.21 |
| ATOM | 1290 | C   | GLU | A | 176 | 18.075 | -16.657 | 45.225 | 1.000 | 35.17 |
| ATOM | 1291 | O   | GLU | A | 176 | 18.353 | -17.212 | 46.288 | 1.000 | 48.02 |
| ATOM | 1292 | N   | SER | A | 177 | 18.794 | -15.685 | 44.683 | 1.000 | 30.91 |
| ATOM | 1293 | CA  | SER | A | 177 | 20.036 | -15.232 | 45.282 | 1.000 | 28.08 |
| ATOM | 1294 | CB  | SER | A | 177 | 21.182 | -15.290 | 44.263 | 1.000 | 26.33 |
| ATOM | 1295 | OG  | SER | A | 177 | 21.340 | -16.639 | 43.844 | 1.000 | 59.53 |
| ATOM | 1296 | C   | SER | A | 177 | 19.908 | -13.811 | 45.804 | 1.000 | 28.71 |
| ATOM | 1297 | O   | SER | A | 177 | 19.678 | -12.900 | 45.008 | 1.000 | 21.80 |
| ATOM | 1298 | N   | VAL | A | 178 | 20.078 | -13.672 | 47.112 | 1.000 | 28.75 |
| ATOM | 1299 | CA  | VAL | A | 178 | 20.081 | -12.360 | 47.739 | 1.000 | 33.94 |

**FIGURE 31**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1300 | CB  | VAL | A | 178 | 19.564 | -12.385 | 49.185 | 1.000 | 36.90 |
| ATOM | 1301 | CG1 | VAL | A | 178 | 19.530 | -10.966 | 49.740 | 1.000 | 26.11 |
| ATOM | 1302 | CG2 | VAL | A | 178 | 18.191 | -13.032 | 49.252 | 1.000 | 38.71 |
| ATOM | 1303 | C   | VAL | A | 178 | 21.492 | -11.768 | 47.753 | 1.000 | 37.69 |
| ATOM | 1304 | O   | VAL | A | 178 | 22.404 | -12.390 | 48.298 | 1.000 | 42.82 |
| ATOM | 1305 | N   | LEU | A | 179 | 21.605 | -10.603 | 47.149 | 1.000 | 36.54 |
| ATOM | 1306 | CA  | LEU | A | 179 | 22.772 | -9.738  | 47.125 | 1.000 | 37.72 |
| ATOM | 1307 | CB  | LEU | A | 179 | 23.086 | -9.250  | 45.709 | 1.000 | 40.59 |
| ATOM | 1308 | CG  | LEU | A | 179 | 23.817 | -10.254 | 44.811 | 1.000 | 42.47 |
| ATOM | 1309 | CD1 | LEU | A | 179 | 24.258 | -11.454 | 45.634 | 1.000 | 49.20 |
| ATOM | 1310 | CD2 | LEU | A | 179 | 22.942 | -10.672 | 43.638 | 1.000 | 27.98 |
| ATOM | 1311 | C   | LEU | A | 179 | 22.522 | -8.547  | 48.041 | 1.000 | 36.64 |
| ATOM | 1312 | O   | LEU | A | 179 | 21.375 | -8.338  | 48.461 | 1.000 | 39.97 |
| ATOM | 1313 | N   | PRO | A | 180 | 23.523 | -7.750  | 48.377 | 1.000 | 35.66 |
| ATOM | 1314 | CA  | PRO | A | 180 | 23.219 | -6.610  | 49.254 | 1.000 | 37.77 |
| ATOM | 1315 | CB  | PRO | A | 180 | 24.584 | -5.934  | 49.447 | 1.000 | 38.49 |
| ATOM | 1316 | CG  | PRO | A | 180 | 25.553 | -7.049  | 49.201 | 1.000 | 37.57 |
| ATOM | 1317 | CD  | PRO | A | 180 | 24.950 | -7.802  | 48.031 | 1.000 | 30.63 |
| ATOM | 1318 | C   | PRO | A | 180 | 22.228 | -5.644  | 48.617 | 1.000 | 33.86 |
| ATOM | 1319 | O   | PRO | A | 180 | 21.382 | -5.100  | 49.338 | 1.000 | 33.02 |
| ATOM | 1320 | N   | GLU | A | 181 | 22.328 | -5.430  | 47.303 | 1.000 | 29.48 |
| ATOM | 1321 | CA  | GLU | A | 181 | 21.557 | -4.357  | 46.678 | 1.000 | 30.49 |
| ATOM | 1322 | CB  | GLU | A | 181 | 22.501 | -3.428  | 45.911 | 1.000 | 33.66 |
| ATOM | 1323 | CG  | GLU | A | 181 | 23.039 | -2.275  | 46.752 | 1.000 | 42.87 |
| ATOM | 1324 | CD  | GLU | A | 181 | 24.282 | -1.678  | 46.120 | 1.000 | 51.54 |
| ATOM | 1325 | OE1 | GLU | A | 181 | 25.233 | -2.443  | 45.850 | 1.000 | 75.46 |
| ATOM | 1326 | OE2 | GLU | A | 181 | 24.303 | -0.455  | 45.890 | 1.000 | 75.08 |
| ATOM | 1327 | C   | GLU | A | 181 | 20.471 | -4.855  | 45.741 | 1.000 | 31.78 |
| ATOM | 1328 | O   | GLU | A | 181 | 19.651 | -4.082  | 45.245 | 1.000 | 30.15 |
| ATOM | 1329 | N   | TRP | A | 182 | 20.469 | -6.158  | 45.486 | 1.000 | 30.83 |
| ATOM | 1330 | CA  | TRP | A | 182 | 19.412 | -6.733  | 44.667 | 1.000 | 29.29 |
| ATOM | 1331 | CB  | TRP | A | 182 | 19.582 | -6.376  | 43.197 | 1.000 | 28.58 |
| ATOM | 1332 | CG  | TRP | A | 182 | 20.858 | -6.827  | 42.567 | 1.000 | 33.11 |
| ATOM | 1333 | CD1 | TRP | A | 182 | 21.167 | -8.066  | 42.078 | 1.000 | 32.78 |
| ATOM | 1334 | NE1 | TRP | A | 182 | 22.451 | -8.067  | 41.577 | 1.000 | 29.50 |
| ATOM | 1335 | CE2 | TRP | A | 182 | 22.991 | -6.819  | 41.738 | 1.000 | 29.38 |
| ATOM | 1336 | CD2 | TRP | A | 182 | 22.021 | -6.010  | 42.354 | 1.000 | 28.84 |
| ATOM | 1337 | CE3 | TRP | A | 182 | 22.313 | -4.676  | 42.637 | 1.000 | 26.83 |
| ATOM | 1338 | CZ3 | TRP | A | 182 | 23.561 | -4.198  | 42.293 | 1.000 | 27.97 |
| ATOM | 1339 | CH2 | TRP | A | 182 | 24.508 | -5.021  | 41.679 | 1.000 | 32.03 |
| ATOM | 1340 | CZ2 | TRP | A | 182 | 24.250 | -6.333  | 41.391 | 1.000 | 35.86 |
| ATOM | 1341 | C   | TRP | A | 182 | 19.363 | -8.248  | 44.842 | 1.000 | 29.75 |
| ATOM | 1342 | O   | TRP | A | 182 | 20.270 | -8.854  | 45.409 | 1.000 | 29.69 |
| ATOM | 1343 | N   | THR | A | 183 | 18.273 | -8.804  | 44.338 | 1.000 | 23.29 |
| ATOM | 1344 | CA  | THR | A | 183 | 17.984 | -10.221 | 44.437 | 1.000 | 22.15 |
| ATOM | 1345 | CB  | THR | A | 183 | 16.812 | -10.506 | 45.397 | 1.000 | 23.41 |
| ATOM | 1346 | OG1 | THR | A | 183 | 17.155 | -10.024 | 46.694 | 1.000 | 26.52 |
| ATOM | 1347 | CG2 | THR | A | 183 | 16.567 | -12.004 | 45.501 | 1.000 | 25.62 |
| ATOM | 1348 | C   | THR | A | 183 | 17.630 | -10.771 | 43.063 | 1.000 | 22.12 |
| ATOM | 1349 | O   | THR | A | 183 | 16.748 | -10.228 | 42.399 | 1.000 | 27.35 |
| ATOM | 1350 | N   | ILE | A | 184 | 18.333 | -11.820 | 42.662 | 1.000 | 22.30 |
| ATOM | 1351 | CA  | ILE | A | 184 | 18.088 | -12.437 | 41.360 | 1.000 | 23.94 |

**FIGURE 32**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1352 | CB  | ILE | A | 184 | 19.396 | -12.675 | 40.592 | 1.000 | 25.30 |
| ATOM | 1353 | CG1 | ILE | A | 184 | 20.199 | -11.396 | 40.326 | 1.000 | 22.21 |
| ATOM | 1354 | CD1 | ILE | A | 184 | 21.601 | -11.696 | 39.831 | 1.000 | 22.92 |
| ATOM | 1355 | CG2 | ILE | A | 184 | 19.170 | -13.392 | 39.270 | 1.000 | 24.72 |
| ATOM | 1356 | C   | ILE | A | 184 | 17.317 | -13.730 | 41.564 | 1.000 | 27.42 |
| ATOM | 1357 | O   | ILE | A | 184 | 17.775 | -14.657 | 42.235 | 1.000 | 27.72 |
| ATOM | 1358 | N   | ARG | A | 185 | 16.108 | -13.816 | 41.000 | 1.000 | 24.23 |
| ATOM | 1359 | CA  | ARG | A | 185 | 15.404 | -15.097 | 41.120 | 1.000 | 17.59 |
| ATOM | 1360 | CB  | ARG | A | 185 | 14.007 | -14.943 | 41.706 | 1.000 | 21.98 |
| ATOM | 1361 | CG  | ARG | A | 185 | 13.946 | -14.608 | 43.191 | 1.000 | 30.13 |
| ATOM | 1362 | CD  | ARG | A | 185 | 12.698 | -13.806 | 43.506 | 1.000 | 29.20 |
| ATOM | 1363 | NE  | ARG | A | 185 | 12.608 | -13.366 | 44.885 | 1.000 | 25.63 |
| ATOM | 1364 | CZ  | ARG | A | 185 | 12.669 | -12.112 | 45.309 | 1.000 | 25.06 |
| ATOM | 1365 | NH1 | ARG | A | 185 | 12.832 | -11.112 | 44.455 | 1.000 | 24.55 |
| ATOM | 1366 | NH2 | ARG | A | 185 | 12.570 | -11.850 | 46.607 | 1.000 | 24.44 |
| ATOM | 1367 | C   | ARG | A | 185 | 15.324 | -15.729 | 39.740 | 1.000 | 18.32 |
| ATOM | 1368 | O   | ARG | A | 185 | 15.468 | -15.034 | 38.737 | 1.000 | 27.89 |
| ATOM | 1369 | N   | GLU | A | 186 | 15.083 | -17.033 | 39.702 | 1.000 | 27.54 |
| ATOM | 1370 | CA  | GLU | A | 186 | 14.806 | -17.688 | 38.433 | 1.000 | 33.52 |
| ATOM | 1371 | CB  | GLU | A | 186 | 15.931 | -18.640 | 38.027 | 1.000 | 37.26 |
| ATOM | 1372 | CG  | GLU | A | 186 | 15.709 | -19.229 | 36.633 | 1.000 | 44.30 |
| ATOM | 1373 | CD  | GLU | A | 186 | 16.999 | -19.785 | 36.063 | 1.000 | 50.45 |
| ATOM | 1374 | OE1 | GLU | A | 186 | 16.974 | -20.303 | 34.930 | 1.000 | 68.14 |
| ATOM | 1375 | OE2 | GLU | A | 186 | 18.035 | -19.694 | 36.755 | 1.000 | 45.57 |
| ATOM | 1376 | C   | GLU | A | 186 | 13.496 | -18.471 | 38.501 | 1.000 | 35.05 |
| ATOM | 1377 | O   | GLU | A | 186 | 13.271 | -19.227 | 39.448 | 1.000 | 27.73 |
| ATOM | 1378 | N   | PHE | A | 187 | 12.649 | -18.294 | 37.488 | 1.000 | 21.89 |
| ATOM | 1379 | CA  | PHE | A | 187 | 11.434 | -19.091 | 37.427 | 1.000 | 24.39 |
| ATOM | 1380 | CB  | PHE | A | 187 | 10.188 | -18.203 | 37.533 | 1.000 | 26.13 |
| ATOM | 1381 | CG  | PHE | A | 187 | 10.245 | -17.205 | 38.663 | 1.000 | 34.20 |
| ATOM | 1382 | CD1 | PHE | A | 187 | 10.669 | -15.907 | 38.444 | 1.000 | 31.66 |
| ATOM | 1383 | CE1 | PHE | A | 187 | 10.727 | -14.979 | 39.465 | 1.000 | 27.66 |
| ATOM | 1384 | CZ  | PHE | A | 187 | 10.352 | -15.353 | 40.737 | 1.000 | 25.23 |
| ATOM | 1385 | CE2 | PHE | A | 187 | 9.926  | -16.645 | 40.980 | 1.000 | 26.99 |
| ATOM | 1386 | CD2 | PHE | A | 187 | 9.875  | -17.565 | 39.952 | 1.000 | 33.63 |
| ATOM | 1387 | C   | PHE | A | 187 | 11.345 | -19.910 | 36.138 | 1.000 | 22.76 |
| ATOM | 1388 | O   | PHE | A | 187 | 11.934 | -19.600 | 35.113 | 1.000 | 22.84 |
| ATOM | 1389 | N   | LYS | A | 188 | 10.568 | -20.964 | 36.254 | 1.000 | 24.79 |
| ATOM | 1390 | CA  | LYS | A | 188 | 10.099 | -21.834 | 35.200 | 1.000 | 26.88 |
| ATOM | 1391 | CB  | LYS | A | 188 | 10.353 | -23.309 | 35.515 | 1.000 | 29.96 |
| ATOM | 1392 | CG  | LYS | A | 188 | 10.069 | -24.234 | 34.340 | 1.000 | 40.94 |
| ATOM | 1393 | CD  | LYS | A | 188 | 10.185 | -25.699 | 34.726 | 1.000 | 36.57 |
| ATOM | 1394 | CE  | LYS | A | 188 | 8.857  | -26.229 | 35.244 | 1.000 | 36.18 |
| ATOM | 1395 | NZ  | LYS | A | 188 | 9.078  | -27.265 | 36.298 | 1.000 | 55.70 |
| ATOM | 1396 | C   | LYS | A | 188 | 8.602  | -21.591 | 35.044 | 1.000 | 24.40 |
| ATOM | 1397 | O   | LYS | A | 188 | 7.885  | -21.601 | 36.049 | 1.000 | 27.61 |
| ATOM | 1398 | N   | ILE | A | 189 | 8.141  | -21.364 | 33.822 | 1.000 | 23.95 |
| ATOM | 1399 | CA  | ILE | A | 189 | 6.710  | -21.109 | 33.659 | 1.000 | 28.81 |
| ATOM | 1400 | CB  | ILE | A | 189 | 6.449  | -19.639 | 33.313 | 1.000 | 35.20 |
| ATOM | 1401 | CG1 | ILE | A | 189 | 4.972  | -19.306 | 33.080 | 1.000 | 43.59 |
| ATOM | 1402 | CD1 | ILE | A | 189 | 4.692  | -17.815 | 33.127 | 1.000 | 51.14 |
| ATOM | 1403 | CG2 | ILE | A | 189 | 7.290  | -19.208 | 32.121 | 1.000 | 19.65 |

**FIGURE 33**

|      |      |     |     |   |     |        |         |        |       |        |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|--------|
| ATOM | 1404 | C   | ILE | A | 189 | 6.141  | -22.040 | 32.594 | 1.000 | 30.63  |
| ATOM | 1405 | O   | ILE | A | 189 | 6.820  | -22.278 | 31.600 | 1.000 | 34.60  |
| ATOM | 1406 | N   | CYS | A | 190 | 4.945  | -22.551 | 32.839 | 1.000 | 36.44  |
| ATOM | 1407 | CA  | CYS | A | 190 | 4.195  | -23.466 | 32.001 | 1.000 | 38.23  |
| ATOM | 1408 | CB  | CYS | A | 190 | 3.935  | -24.832 | 32.645 | 1.000 | 36.83  |
| ATOM | 1409 | SG  | CYS | A | 190 | 5.333  | -25.621 | 33.465 | 1.000 | 54.28  |
| ATOM | 1410 | C   | CYS | A | 190 | 2.836  | -22.854 | 31.647 | 1.000 | 40.07  |
| ATOM | 1411 | O   | CYS | A | 190 | 2.035  | -22.528 | 32.524 | 1.000 | 34.54  |
| ATOM | 1412 | N   | GLY | A | 191 | 2.596  | -22.714 | 30.348 | 1.000 | 38.67  |
| ATOM | 1413 | CA  | GLY | A | 191 | 1.317  | -22.192 | 29.891 | 1.000 | 47.19  |
| ATOM | 1414 | C   | GLY | A | 191 | 0.665  | -23.168 | 28.937 | 1.000 | 57.83  |
| ATOM | 1415 | O   | GLY | A | 191 | 1.108  | -24.313 | 28.810 | 1.000 | 57.59  |
| ATOM | 1416 | N   | GLU | A | 192 | -0.394 | -22.733 | 28.252 | 1.000 | 68.94  |
| ATOM | 1417 | CA  | GLU | A | 192 | -0.950 | -23.669 | 27.264 | 1.000 | 77.08  |
| ATOM | 1418 | CB  | GLU | A | 192 | -2.249 | -23.139 | 26.671 | 1.000 | 79.72  |
| ATOM | 1419 | CG  | GLU | A | 192 | -3.488 | -23.931 | 27.082 | 1.000 | 83.44  |
| ATOM | 1420 | CD  | GLU | A | 192 | -4.763 | -23.113 | 27.103 | 1.000 | 88.99  |
| ATOM | 1421 | OE1 | GLU | A | 192 | -4.760 | -21.996 | 27.669 | 1.000 | 97.81  |
| ATOM | 1422 | OE2 | GLU | A | 192 | -5.784 | -23.582 | 26.555 | 1.000 | 83.85  |
| ATOM | 1423 | C   | GLU | A | 192 | 0.137  | -23.932 | 26.222 | 1.000 | 79.08  |
| ATOM | 1424 | O   | GLU | A | 192 | 0.449  | -23.046 | 25.419 | 1.000 | 84.98  |
| ATOM | 1425 | N   | GLU | A | 193 | 0.712  | -25.136 | 26.276 | 1.000 | 80.23  |
| ATOM | 1426 | CA  | GLU | A | 193 | 1.810  | -25.537 | 25.407 | 1.000 | 88.15  |
| ATOM | 1427 | CB  | GLU | A | 193 | 1.859  | -27.061 | 25.268 | 1.000 | 82.57  |
| ATOM | 1428 | CG  | GLU | A | 193 | 2.981  | -27.559 | 24.373 | 1.000 | 74.69  |
| ATOM | 1429 | CD  | GLU | A | 193 | 4.340  | -27.361 | 25.023 | 1.000 | 75.38  |
| ATOM | 1430 | OE1 | GLU | A | 193 | 4.581  | -27.990 | 26.075 | 1.000 | 64.29  |
| ATOM | 1431 | OE2 | GLU | A | 193 | 5.153  | -26.581 | 24.488 | 1.000 | 79.60  |
| ATOM | 1432 | C   | GLU | A | 193 | 1.682  | -24.896 | 24.026 | 1.000 | 100.09 |
| ATOM | 1433 | O   | GLU | A | 193 | 0.956  | -25.403 | 23.166 | 1.000 | 118.96 |
| ATOM | 1434 | N   | GLN | A | 194 | 2.383  | -23.782 | 23.814 | 1.000 | 102.10 |
| ATOM | 1435 | CA  | GLN | A | 194 | 2.277  | -23.101 | 22.520 | 1.000 | 107.47 |
| ATOM | 1436 | CB  | GLN | A | 194 | 1.451  | -21.819 | 22.686 | 1.000 | 110.48 |
| ATOM | 1437 | CG  | GLN | A | 194 | 0.039  | -22.092 | 23.245 | 1.000 | 111.93 |
| ATOM | 1438 | CD  | GLN | A | 194 | -0.952 | -20.989 | 22.858 | 1.000 | 112.96 |
| ATOM | 1439 | OE1 | GLN | A | 194 | -0.959 | -20.485 | 21.724 | 1.000 | 119.77 |
| ATOM | 1440 | NE2 | GLN | A | 194 | -1.812 | -20.629 | 23.805 | 1.000 | 105.14 |
| ATOM | 1441 | C   | GLN | A | 194 | 3.653  | -22.834 | 21.928 | 1.000 | 110.55 |
| ATOM | 1442 | O   | GLN | A | 194 | 4.374  | -23.775 | 21.570 | 1.000 | 118.12 |
| ATOM | 1443 | N   | LEU | A | 195 | 4.067  | -21.573 | 21.796 | 1.000 | 108.99 |
| ATOM | 1444 | CA  | LEU | A | 195 | 5.409  | -21.363 | 21.238 | 1.000 | 106.04 |
| ATOM | 1445 | CB  | LEU | A | 195 | 5.601  | -19.930 | 20.752 | 1.000 | 103.44 |
| ATOM | 1446 | CG  | LEU | A | 195 | 6.025  | -19.764 | 19.285 | 1.000 | 101.76 |
| ATOM | 1447 | CD1 | LEU | A | 195 | 6.636  | -18.390 | 19.041 | 1.000 | 93.51  |
| ATOM | 1448 | CD2 | LEU | A | 195 | 7.000  | -20.865 | 18.871 | 1.000 | 83.67  |
| ATOM | 1449 | C   | LEU | A | 195 | 6.462  | -21.736 | 22.276 | 1.000 | 109.72 |
| ATOM | 1450 | O   | LEU | A | 195 | 7.662  | -21.740 | 21.977 | 1.000 | 128.83 |
| ATOM | 1451 | N   | ASP | A | 196 | 6.020  | -22.054 | 23.495 | 1.000 | 104.75 |
| ATOM | 1452 | CA  | ASP | A | 196 | 6.956  | -22.505 | 24.521 | 1.000 | 97.46  |
| ATOM | 1453 | CB  | ASP | A | 196 | 7.139  | -21.463 | 25.616 | 1.000 | 94.37  |
| ATOM | 1454 | CG  | ASP | A | 196 | 6.470  | -20.133 | 25.358 | 1.000 | 89.89  |
| ATOM | 1455 | OD1 | ASP | A | 196 | 5.236  | -20.089 | 25.182 | 1.000 | 80.93  |

**FIGURE 34**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |       |        |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|--------|
| ATOM | 1456 | OD2 | ASP | A | 196 | 7.206  | -19.119 | 25.348 | 1.000 | 73.17  |
| ATOM | 1457 | C   | ASP | A | 196 | 6.498  | -23.822 | 25.150 | 1.000 | 96.72  |
| ATOM | 1458 | O   | ASP | A | 196 | 5.391  | -24.300 | 24.896 | 1.000 | 103.69 |
| ATOM | 1459 | N   | ALA | A | 197 | 7.366  | -24.390 | 25.976 | 1.000 | 95.34  |
| ATOM | 1460 | CA  | ALA | A | 197 | 7.113  | -25.628 | 26.703 | 1.000 | 92.76  |
| ATOM | 1461 | CB  | ALA | A | 197 | 7.661  | -26.824 | 25.949 | 1.000 | 80.95  |
| ATOM | 1462 | C   | ALA | A | 197 | 7.715  | -25.535 | 28.106 | 1.000 | 92.67  |
| ATOM | 1463 | O   | ALA | A | 197 | 6.986  | -25.567 | 29.100 | 1.000 | 101.36 |
| ATOM | 1464 | N   | HIS | A | 198 | 9.035  | -25.410 | 28.190 | 1.000 | 90.04  |
| ATOM | 1465 | CA  | HIS | A | 198 | 9.720  | -25.190 | 29.464 | 1.000 | 83.32  |
| ATOM | 1466 | CB  | HIS | A | 198 | 10.618 | -26.370 | 29.813 | 1.000 | 84.18  |
| ATOM | 1467 | CG  | HIS | A | 198 | 11.844 | -26.074 | 30.617 | 1.000 | 84.25  |
| ATOM | 1468 | ND1 | HIS | A | 198 | 11.839 | -25.834 | 31.968 | 1.000 | 86.44  |
| ATOM | 1469 | CE1 | HIS | A | 198 | 13.071 | -25.609 | 32.389 | 1.000 | 85.15  |
| ATOM | 1470 | NE2 | HIS | A | 198 | 13.884 | -25.681 | 31.348 | 1.000 | 81.36  |
| ATOM | 1471 | CD2 | HIS | A | 198 | 13.141 | -25.969 | 30.232 | 1.000 | 81.88  |
| ATOM | 1472 | C   | HIS | A | 198 | 10.489 | -23.876 | 29.379 | 1.000 | 70.03  |
| ATOM | 1473 | O   | HIS | A | 198 | 11.664 | -23.784 | 29.023 | 1.000 | 64.25  |
| ATOM | 1474 | N   | ARG | A | 199 | 9.790  | -22.781 | 29.701 | 1.000 | 58.16  |
| ATOM | 1475 | CA  | ARG | A | 199 | 10.431 | -21.480 | 29.568 | 1.000 | 50.11  |
| ATOM | 1476 | CB  | ARG | A | 199 | 9.498  | -20.464 | 28.903 | 1.000 | 50.90  |
| ATOM | 1477 | CG  | ARG | A | 199 | 10.292 | -19.446 | 28.092 | 1.000 | 53.59  |
| ATOM | 1478 | CD  | ARG | A | 199 | 9.616  | -18.087 | 28.108 | 1.000 | 48.39  |
| ATOM | 1479 | NE  | ARG | A | 199 | 8.377  | -18.120 | 27.322 | 1.000 | 42.37  |
| ATOM | 1480 | CZ  | ARG | A | 199 | 7.502  | -17.120 | 27.427 | 1.000 | 43.29  |
| ATOM | 1481 | NH1 | ARG | A | 199 | 7.751  | -16.096 | 28.241 | 1.000 | 31.50  |
| ATOM | 1482 | NH2 | ARG | A | 199 | 6.398  | -17.186 | 26.709 | 1.000 | 24.97  |
| ATOM | 1483 | C   | ARG | A | 199 | 10.900 | -20.944 | 30.918 | 1.000 | 37.10  |
| ATOM | 1484 | O   | ARG | A | 199 | 10.201 | -21.106 | 31.914 | 1.000 | 28.73  |
| ATOM | 1485 | N   | LEU | A | 200 | 12.079 | -20.336 | 30.889 | 1.000 | 29.92  |
| ATOM | 1486 | CA  | LEU | A | 200 | 12.757 | -19.865 | 32.087 | 1.000 | 35.35  |
| ATOM | 1487 | CB  | LEU | A | 200 | 14.196 | -20.394 | 32.149 | 1.000 | 38.39  |
| ATOM | 1488 | CG  | LEU | A | 200 | 14.295 | -21.881 | 32.511 | 1.000 | 51.57  |
| ATOM | 1489 | CD1 | LEU | A | 200 | 15.401 | -22.134 | 33.523 | 1.000 | 73.84  |
| ATOM | 1490 | CD2 | LEU | A | 200 | 12.963 | -22.382 | 33.052 | 1.000 | 69.62  |
| ATOM | 1491 | C   | LEU | A | 200 | 12.762 | -18.343 | 32.153 | 1.000 | 31.71  |
| ATOM | 1492 | O   | LEU | A | 200 | 13.040 | -17.681 | 31.155 | 1.000 | 29.83  |
| ATOM | 1493 | N   | ILE | A | 201 | 12.446 | -17.820 | 33.333 | 1.000 | 23.61  |
| ATOM | 1494 | CA  | ILE | A | 201 | 12.371 | -16.376 | 33.510 | 1.000 | 23.62  |
| ATOM | 1495 | CB  | ILE | A | 201 | 10.962 | -15.892 | 33.903 | 1.000 | 25.57  |
| ATOM | 1496 | CG1 | ILE | A | 201 | 9.858  | -16.232 | 32.898 | 1.000 | 30.41  |
| ATOM | 1497 | CD1 | ILE | A | 201 | 10.310 | -16.192 | 31.459 | 1.000 | 26.58  |
| ATOM | 1498 | CG2 | ILE | A | 201 | 10.964 | -14.395 | 34.171 | 1.000 | 23.03  |
| ATOM | 1499 | C   | ILE | A | 201 | 13.332 | -15.933 | 34.604 | 1.000 | 22.99  |
| ATOM | 1500 | O   | ILE | A | 201 | 13.382 | -16.507 | 35.688 | 1.000 | 27.49  |
| ATOM | 1501 | N   | ARG | A | 202 | 14.088 | -14.886 | 34.299 | 1.000 | 19.58  |
| ATOM | 1502 | CA  | ARG | A | 202 | 14.960 | -14.324 | 35.320 | 1.000 | 17.66  |
| ATOM | 1503 | CB  | ARG | A | 202 | 16.361 | -14.091 | 34.768 | 1.000 | 25.08  |
| ATOM | 1504 | CG  | ARG | A | 202 | 17.450 | -14.797 | 35.562 | 1.000 | 39.27  |
| ATOM | 1505 | CD  | ARG | A | 202 | 18.605 | -15.183 | 34.654 | 1.000 | 48.88  |
| ATOM | 1506 | NE  | ARG | A | 202 | 19.385 | -16.289 | 35.220 | 1.000 | 55.89  |
| ATOM | 1507 | CZ  | ARG | A | 202 | 19.961 | -17.201 | 34.435 | 1.000 | 60.48  |

**FIGURE 35**

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1508 | NH1 | ARG | A | 202 | 19.812 | -17.100 | 33.119 | 1.000 | 50.30 |
| ATOM | 1509 | NH2 | ARG | A | 202 | 20.666 | -18.191 | 34.965 | 1.000 | 77.85 |
| ATOM | 1510 | C   | ARG | A | 202 | 14.343 | -13.023 | 35.826 | 1.000 | 22.83 |
| ATOM | 1511 | O   | ARG | A | 202 | 13.885 | -12.219 | 35.007 | 1.000 | 22.73 |
| ATOM | 1512 | N   | HIS | A | 203 | 14.345 | -12.858 | 37.136 | 1.000 | 18.38 |
| ATOM | 1513 | CA  | HIS | A | 203 | 13.794 | -11.690 | 37.815 | 1.000 | 21.09 |
| ATOM | 1514 | CB  | HIS | A | 203 | 12.701 | -12.145 | 38.770 | 1.000 | 22.13 |
| ATOM | 1515 | CG  | HIS | A | 203 | 11.824 | -11.117 | 39.389 | 1.000 | 24.48 |
| ATOM | 1516 | ND1 | HIS | A | 203 | 12.146 | -10.463 | 40.554 | 1.000 | 20.07 |
| ATOM | 1517 | CE1 | HIS | A | 203 | 11.186 | -9.616  | 40.875 | 1.000 | 23.08 |
| ATOM | 1518 | NE2 | HIS | A | 203 | 10.240 | -9.697  | 39.959 | 1.000 | 27.63 |
| ATOM | 1519 | CD2 | HIS | A | 203 | 10.611 | -10.629 | 39.022 | 1.000 | 25.25 |
| ATOM | 1520 | C   | HIS | A | 203 | 14.894 | -10.952 | 38.579 | 1.000 | 27.02 |
| ATOM | 1521 | O   | HIS | A | 203 | 15.541 | -11.548 | 39.447 | 1.000 | 18.53 |
| ATOM | 1522 | N   | PHE | A | 204 | 15.086 | -9.691  | 38.246 | 1.000 | 21.78 |
| ATOM | 1523 | CA  | PHE | A | 204 | 16.068 | -8.796  | 38.840 | 1.000 | 16.28 |
| ATOM | 1524 | CB  | PHE | A | 204 | 16.891 | -8.101  | 37.742 | 1.000 | 16.39 |
| ATOM | 1525 | CG  | PHE | A | 204 | 17.526 | -9.112  | 36.813 | 1.000 | 27.16 |
| ATOM | 1526 | CD1 | PHE | A | 204 | 16.899 | -9.466  | 35.632 | 1.000 | 16.95 |
| ATOM | 1527 | CE1 | PHE | A | 204 | 17.476 | -10.397 | 34.790 | 1.000 | 26.09 |
| ATOM | 1528 | CZ  | PHE | A | 204 | 18.686 | -10.979 | 35.123 | 1.000 | 31.27 |
| ATOM | 1529 | CE2 | PHE | A | 204 | 19.326 | -10.639 | 36.303 | 1.000 | 26.75 |
| ATOM | 1530 | CD2 | PHE | A | 204 | 18.744 | -9.699  | 37.136 | 1.000 | 28.81 |
| ATOM | 1531 | C   | PHE | A | 204 | 15.378 | -7.752  | 39.707 | 1.000 | 16.41 |
| ATOM | 1532 | O   | PHE | A | 204 | 14.748 | -6.809  | 39.223 | 1.000 | 24.46 |
| ATOM | 1533 | N   | HIS | A | 205 | 15.514 | -7.930  | 41.006 | 1.000 | 16.66 |
| ATOM | 1534 | CA  | HIS | A | 205 | 14.879 | -7.081  | 41.998 | 1.000 | 14.51 |
| ATOM | 1535 | CB  | HIS | A | 205 | 14.118 | -7.987  | 42.982 | 1.000 | 14.31 |
| ATOM | 1536 | CG  | HIS | A | 205 | 13.201 | -7.221  | 43.887 | 1.000 | 25.21 |
| ATOM | 1537 | ND1 | HIS | A | 205 | 12.631 | -7.784  | 45.009 | 1.000 | 24.28 |
| ATOM | 1538 | CE1 | HIS | A | 205 | 11.882 | -6.885  | 45.611 | 1.000 | 27.88 |
| ATOM | 1539 | NE2 | HIS | A | 205 | 11.939 | -5.756  | 44.927 | 1.000 | 24.25 |
| ATOM | 1540 | CD2 | HIS | A | 205 | 12.761 | -5.949  | 43.845 | 1.000 | 28.00 |
| ATOM | 1541 | C   | HIS | A | 205 | 15.867 | -6.211  | 42.764 | 1.000 | 26.42 |
| ATOM | 1542 | O   | HIS | A | 205 | 16.535 | -6.668  | 43.697 | 1.000 | 21.37 |
| ATOM | 1543 | N   | TYR | A | 206 | 15.950 | -4.954  | 42.359 | 1.000 | 25.43 |
| ATOM | 1544 | CA  | TYR | A | 206 | 16.705 | -3.918  | 43.045 | 1.000 | 26.77 |
| ATOM | 1545 | CB  | TYR | A | 206 | 16.849 | -2.707  | 42.142 | 1.000 | 30.54 |
| ATOM | 1546 | CG  | TYR | A | 206 | 17.810 | -1.643  | 42.603 | 1.000 | 30.50 |
| ATOM | 1547 | CD1 | TYR | A | 206 | 19.177 | -1.758  | 42.349 | 1.000 | 21.06 |
| ATOM | 1548 | CE1 | TYR | A | 206 | 20.048 | -0.774  | 42.779 | 1.000 | 26.02 |
| ATOM | 1549 | CZ  | TYR | A | 206 | 19.551 | 0.320   | 43.457 | 1.000 | 28.32 |
| ATOM | 1550 | OH  | TYR | A | 206 | 20.406 | 1.309   | 43.883 | 1.000 | 33.26 |
| ATOM | 1551 | CE2 | TYR | A | 206 | 18.201 | 0.452   | 43.715 | 1.000 | 31.83 |
| ATOM | 1552 | CD2 | TYR | A | 206 | 17.330 | -0.534  | 43.289 | 1.000 | 30.09 |
| ATOM | 1553 | C   | TYR | A | 206 | 15.978 | -3.521  | 44.324 | 1.000 | 32.60 |
| ATOM | 1554 | O   | TYR | A | 206 | 14.893 | -2.942  | 44.266 | 1.000 | 27.05 |
| ATOM | 1555 | N   | THR | A | 207 | 16.574 | -3.858  | 45.460 | 1.000 | 30.86 |
| ATOM | 1556 | CA  | THR | A | 207 | 15.870 | -3.793  | 46.729 | 1.000 | 34.19 |
| ATOM | 1557 | CB  | THR | A | 207 | 16.205 | -5.071  | 47.535 | 1.000 | 35.60 |
| ATOM | 1558 | OG1 | THR | A | 207 | 17.627 | -5.263  | 47.486 | 1.000 | 37.52 |
| ATOM | 1559 | CG2 | THR | A | 207 | 15.545 | -6.290  | 46.917 | 1.000 | 40.16 |

FIGURE 36



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1560 | C   | THR | A | 207 | 16.214 | -2.599 | 47.604 | 1.000 | 42.95 |
| ATOM | 1561 | O   | THR | A | 207 | 15.790 | -2.560 | 48.768 | 1.000 | 33.25 |
| ATOM | 1562 | N   | VAL | A | 208 | 16.982 | -1.633 | 47.105 | 1.000 | 38.87 |
| ATOM | 1563 | CA  | VAL | A | 208 | 17.495 | -0.587 | 47.986 | 1.000 | 42.20 |
| ATOM | 1564 | CB  | VAL | A | 208 | 19.001 | -0.829 | 48.254 | 1.000 | 38.89 |
| ATOM | 1565 | CG1 | VAL | A | 208 | 19.208 | -2.188 | 48.913 | 1.000 | 29.05 |
| ATOM | 1566 | CG2 | VAL | A | 208 | 19.810 | -0.734 | 46.973 | 1.000 | 32.10 |
| ATOM | 1567 | C   | VAL | A | 208 | 17.304 | 0.826  | 47.464 | 1.000 | 41.85 |
| ATOM | 1568 | O   | VAL | A | 208 | 18.055 | 1.725  | 47.850 | 1.000 | 40.55 |
| ATOM | 1569 | N   | TRP | A | 209 | 16.329 | 1.095  | 46.602 | 1.000 | 38.83 |
| ATOM | 1570 | CA  | TRP | A | 209 | 16.039 | 2.473  | 46.199 | 1.000 | 36.12 |
| ATOM | 1571 | CB  | TRP | A | 209 | 15.037 | 2.480  | 45.053 | 1.000 | 31.43 |
| ATOM | 1572 | CG  | TRP | A | 209 | 15.042 | 3.683  | 44.170 | 1.000 | 31.44 |
| ATOM | 1573 | CD1 | TRP | A | 209 | 14.710 | 4.963  | 44.509 | 1.000 | 26.97 |
| ATOM | 1574 | NE1 | TRP | A | 209 | 14.840 | 5.788  | 43.417 | 1.000 | 29.65 |
| ATOM | 1575 | CE2 | TRP | A | 209 | 15.261 | 5.047  | 42.342 | 1.000 | 23.71 |
| ATOM | 1576 | CD2 | TRP | A | 209 | 15.399 | 3.717  | 42.779 | 1.000 | 28.34 |
| ATOM | 1577 | CE3 | TRP | A | 209 | 15.821 | 2.749  | 41.862 | 1.000 | 32.82 |
| ATOM | 1578 | CZ3 | TRP | A | 209 | 16.086 | 3.142  | 40.564 | 1.000 | 33.95 |
| ATOM | 1579 | CH2 | TRP | A | 209 | 15.939 | 4.478  | 40.159 | 1.000 | 36.07 |
| ATOM | 1580 | CZ2 | TRP | A | 209 | 15.527 | 5.448  | 41.033 | 1.000 | 22.47 |
| ATOM | 1581 | C   | TRP | A | 209 | 15.490 | 3.239  | 47.397 | 1.000 | 36.81 |
| ATOM | 1582 | O   | TRP | A | 209 | 14.515 | 2.795  | 48.008 | 1.000 | 32.77 |
| ATOM | 1583 | N   | PRO | A | 210 | 16.069 | 4.369  | 47.770 | 1.000 | 34.94 |
| ATOM | 1584 | CA  | PRO | A | 210 | 15.624 | 5.061  | 48.987 | 1.000 | 33.09 |
| ATOM | 1585 | CB  | PRO | A | 210 | 16.456 | 6.345  | 48.988 | 1.000 | 32.95 |
| ATOM | 1586 | CG  | PRO | A | 210 | 17.633 | 6.063  | 48.123 | 1.000 | 34.50 |
| ATOM | 1587 | CD  | PRO | A | 210 | 17.160 | 5.078  | 47.088 | 1.000 | 36.07 |
| ATOM | 1588 | C   | PRO | A | 210 | 14.140 | 5.412  | 48.940 | 1.000 | 41.55 |
| ATOM | 1589 | O   | PRO | A | 210 | 13.515 | 5.321  | 47.882 | 1.000 | 42.95 |
| ATOM | 1590 | N   | ASP | A | 211 | 13.590 | 5.820  | 50.081 | 1.000 | 49.64 |
| ATOM | 1591 | CA  | ASP | A | 211 | 12.183 | 6.214  | 50.158 | 1.000 | 54.78 |
| ATOM | 1592 | CB  | ASP | A | 211 | 11.720 | 6.296  | 51.612 | 1.000 | 55.95 |
| ATOM | 1593 | CG  | ASP | A | 211 | 11.048 | 5.030  | 52.100 | 1.000 | 56.96 |
| ATOM | 1594 | OD1 | ASP | A | 211 | 10.660 | 4.976  | 53.286 | 1.000 | 50.78 |
| ATOM | 1595 | OD2 | ASP | A | 211 | 10.905 | 4.079  | 51.306 | 1.000 | 63.04 |
| ATOM | 1596 | C   | ASP | A | 211 | 11.959 | 7.551  | 49.457 | 1.000 | 52.82 |
| ATOM | 1597 | O   | ASP | A | 211 | 10.896 | 7.882  | 48.937 | 1.000 | 45.02 |
| ATOM | 1598 | N   | HIS | A | 212 | 13.020 | 8.351  | 49.446 | 1.000 | 48.03 |
| ATOM | 1599 | CA  | HIS | A | 212 | 12.961 | 9.675  | 48.845 | 1.000 | 53.87 |
| ATOM | 1600 | CB  | HIS | A | 212 | 12.846 | 10.746 | 49.934 | 1.000 | 72.68 |
| ATOM | 1601 | CG  | HIS | A | 212 | 12.681 | 10.177 | 51.311 | 1.000 | 76.92 |
| ATOM | 1602 | ND1 | HIS | A | 212 | 11.458 | 10.093 | 51.935 | 1.000 | 78.57 |
| ATOM | 1603 | CE1 | HIS | A | 212 | 11.610 | 9.555  | 53.133 | 1.000 | 80.63 |
| ATOM | 1604 | NE2 | HIS | A | 212 | 12.890 | 9.277  | 53.307 | 1.000 | 79.40 |
| ATOM | 1605 | CD2 | HIS | A | 212 | 13.578 | 9.660  | 52.180 | 1.000 | 77.05 |
| ATOM | 1606 | C   | HIS | A | 212 | 14.197 | 9.908  | 47.986 | 1.000 | 46.17 |
| ATOM | 1607 | O   | HIS | A | 212 | 15.310 | 9.572  | 48.392 | 1.000 | 42.06 |
| ATOM | 1608 | N   | GLY | A | 213 | 13.992 | 10.472 | 46.799 | 1.000 | 43.66 |
| ATOM | 1609 | CA  | GLY | A | 213 | 15.091 | 10.704 | 45.885 | 1.000 | 43.27 |
| ATOM | 1610 | C   | GLY | A | 213 | 15.654 | 9.421  | 45.299 | 1.000 | 41.13 |
| ATOM | 1611 | O   | GLY | A | 213 | 15.050 | 8.357  | 45.431 | 1.000 | 31.32 |

**FIGURE 37**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1612 | N   | VAL | A | 214 | 16.804 | 9.569  | 44.663 | 1.000 | 40.78 |
| ATOM | 1613 | CA  | VAL | A | 214 | 17.476 | 8.540  | 43.881 | 1.000 | 37.49 |
| ATOM | 1614 | CB  | VAL | A | 214 | 18.098 | 9.200  | 42.644 | 1.000 | 31.11 |
| ATOM | 1615 | CG1 | VAL | A | 214 | 17.047 | 10.031 | 41.917 | 1.000 | 31.20 |
| ATOM | 1616 | CG2 | VAL | A | 214 | 19.284 | 10.056 | 43.059 | 1.000 | 42.36 |
| ATOM | 1617 | C   | VAL | A | 214 | 18.526 | 7.827  | 44.715 | 1.000 | 45.89 |
| ATOM | 1618 | O   | VAL | A | 214 | 18.953 | 8.384  | 45.729 | 1.000 | 57.46 |
| ATOM | 1619 | N   | PRO | A | 215 | 18.933 | 6.624  | 44.333 | 1.000 | 40.93 |
| ATOM | 1620 | CA  | PRO | A | 215 | 19.764 | 5.782  | 45.188 | 1.000 | 34.00 |
| ATOM | 1621 | CB  | PRO | A | 215 | 20.251 | 4.672  | 44.247 | 1.000 | 42.73 |
| ATOM | 1622 | CG  | PRO | A | 215 | 19.225 | 4.606  | 43.168 | 1.000 | 48.15 |
| ATOM | 1623 | CD  | PRO | A | 215 | 18.636 | 5.975  | 43.041 | 1.000 | 45.87 |
| ATOM | 1624 | C   | PRO | A | 215 | 21.003 | 6.478  | 45.755 | 1.000 | 38.07 |
| ATOM | 1625 | O   | PRO | A | 215 | 21.508 | 7.427  | 45.159 | 1.000 | 36.58 |
| ATOM | 1626 | N   | GLU | A | 216 | 21.427 | 5.942  | 46.886 | 1.000 | 51.41 |
| ATOM | 1627 | CA  | GLU | A | 216 | 22.569 | 6.331  | 47.688 | 1.000 | 59.42 |
| ATOM | 1628 | CB  | GLU | A | 216 | 23.016 | 5.168  | 48.587 | 1.000 | 62.22 |
| ATOM | 1629 | CG  | GLU | A | 216 | 24.008 | 5.566  | 49.666 | 1.000 | 66.95 |
| ATOM | 1630 | CD  | GLU | A | 216 | 25.143 | 4.586  | 49.863 | 1.000 | 69.08 |
| ATOM | 1631 | OE1 | GLU | A | 216 | 24.891 | 3.377  | 50.036 | 1.000 | 49.54 |
| ATOM | 1632 | OE2 | GLU | A | 216 | 26.314 | 5.036  | 49.867 | 1.000 | 70.82 |
| ATOM | 1633 | C   | GLU | A | 216 | 23.739 | 6.782  | 46.818 | 1.000 | 54.66 |
| ATOM | 1634 | O   | GLU | A | 216 | 24.238 | 7.895  | 46.980 | 1.000 | 48.01 |
| ATOM | 1635 | N   | THR | A | 217 | 24.155 | 5.905  | 45.908 | 1.000 | 43.30 |
| ATOM | 1636 | CA  | THR | A | 217 | 25.239 | 6.207  | 44.989 | 1.000 | 40.68 |
| ATOM | 1637 | CB  | THR | A | 217 | 26.492 | 5.353  | 45.264 | 1.000 | 40.90 |
| ATOM | 1638 | OG1 | THR | A | 217 | 26.180 | 3.960  | 45.083 | 1.000 | 41.85 |
| ATOM | 1639 | CG2 | THR | A | 217 | 26.966 | 5.527  | 46.698 | 1.000 | 28.03 |
| ATOM | 1640 | C   | THR | A | 217 | 24.823 | 5.970  | 43.535 | 1.000 | 42.76 |
| ATOM | 1641 | O   | THR | A | 217 | 23.831 | 5.299  | 43.269 | 1.000 | 55.29 |
| ATOM | 1642 | N   | THR | A | 218 | 25.612 | 6.524  | 42.625 | 1.000 | 38.69 |
| ATOM | 1643 | CA  | THR | A | 218 | 25.506 | 6.280  | 41.199 | 1.000 | 46.38 |
| ATOM | 1644 | CB  | THR | A | 218 | 26.407 | 7.242  | 40.399 | 1.000 | 48.77 |
| ATOM | 1645 | OG1 | THR | A | 218 | 27.771 | 7.133  | 40.833 | 1.000 | 31.20 |
| ATOM | 1646 | CG2 | THR | A | 218 | 26.004 | 8.690  | 40.634 | 1.000 | 44.45 |
| ATOM | 1647 | C   | THR | A | 218 | 25.887 | 4.831  | 40.882 | 1.000 | 40.27 |
| ATOM | 1648 | O   | THR | A | 218 | 25.248 | 4.124  | 40.099 | 1.000 | 43.37 |
| ATOM | 1649 | N   | GLN | A | 219 | 26.962 | 4.401  | 41.524 | 1.000 | 36.77 |
| ATOM | 1650 | CA  | GLN | A | 219 | 27.592 | 3.095  | 41.332 | 1.000 | 40.35 |
| ATOM | 1651 | CB  | GLN | A | 219 | 28.841 | 3.052  | 42.215 | 1.000 | 46.27 |
| ATOM | 1652 | CG  | GLN | A | 219 | 29.392 | 1.680  | 42.538 | 1.000 | 60.44 |
| ATOM | 1653 | CD  | GLN | A | 219 | 30.902 | 1.629  | 42.393 | 1.000 | 71.25 |
| ATOM | 1654 | OE1 | GLN | A | 219 | 31.414 | 1.573  | 41.274 | 1.000 | 90.40 |
| ATOM | 1655 | NE2 | GLN | A | 219 | 31.593 | 1.640  | 43.527 | 1.000 | 53.90 |
| ATOM | 1656 | C   | GLN | A | 219 | 26.621 | 1.959  | 41.619 | 1.000 | 37.53 |
| ATOM | 1657 | O   | GLN | A | 219 | 26.618 | 0.907  | 40.977 | 1.000 | 32.61 |
| ATOM | 1658 | N   | SER | A | 220 | 25.739 | 2.146  | 42.596 | 1.000 | 33.04 |
| ATOM | 1659 | CA  | SER | A | 220 | 24.720 | 1.164  | 42.929 | 1.000 | 26.50 |
| ATOM | 1660 | CB  | SER | A | 220 | 23.845 | 1.739  | 44.049 | 1.000 | 29.93 |
| ATOM | 1661 | OG  | SER | A | 220 | 22.837 | 0.814  | 44.413 | 1.000 | 35.63 |
| ATOM | 1662 | C   | SER | A | 220 | 23.860 | 0.792  | 41.727 | 1.000 | 34.98 |
| ATOM | 1663 | O   | SER | A | 220 | 23.745 | -0.378 | 41.354 | 1.000 | 31.36 |

**FIGURE 38**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1664 | N   | LEU | A | 221 | 23.247 | 1.800  | 41.104 | 1.000 | 34.26 |
| ATOM | 1665 | CA  | LEU | A | 221 | 22.404 | 1.571  | 39.940 | 1.000 | 32.25 |
| ATOM | 1666 | CB  | LEU | A | 221 | 21.483 | 2.764  | 39.648 | 1.000 | 25.67 |
| ATOM | 1667 | CG  | LEU | A | 221 | 20.313 | 2.430  | 38.705 | 1.000 | 23.74 |
| ATOM | 1668 | CD1 | LEU | A | 221 | 19.468 | 1.312  | 39.303 | 1.000 | 18.81 |
| ATOM | 1669 | CD2 | LEU | A | 221 | 19.490 | 3.672  | 38.420 | 1.000 | 28.95 |
| ATOM | 1670 | C   | LEU | A | 221 | 23.238 | 1.270  | 38.700 | 1.000 | 36.04 |
| ATOM | 1671 | O   | LEU | A | 221 | 22.797 | 0.534  | 37.806 | 1.000 | 29.22 |
| ATOM | 1672 | N   | ILE | A | 222 | 24.446 | 1.845  | 38.637 | 1.000 | 33.99 |
| ATOM | 1673 | CA  | ILE | A | 222 | 25.231 | 1.532  | 37.445 | 1.000 | 25.77 |
| ATOM | 1674 | CB  | ILE | A | 222 | 26.562 | 2.282  | 37.364 | 1.000 | 24.00 |
| ATOM | 1675 | CG1 | ILE | A | 222 | 26.426 | 3.748  | 36.963 | 1.000 | 25.72 |
| ATOM | 1676 | CD1 | ILE | A | 222 | 27.516 | 4.638  | 37.512 | 1.000 | 30.84 |
| ATOM | 1677 | CG2 | ILE | A | 222 | 27.496 | 1.556  | 36.405 | 1.000 | 31.40 |
| ATOM | 1678 | C   | ILE | A | 222 | 25.511 | 0.027  | 37.382 | 1.000 | 27.84 |
| ATOM | 1679 | O   | ILE | A | 222 | 25.444 | -0.541 | 36.293 | 1.000 | 29.04 |
| ATOM | 1680 | N   | GLN | A | 223 | 25.789 | -0.572 | 38.525 | 1.000 | 25.48 |
| ATOM | 1681 | CA  | GLN | A | 223 | 26.120 | -1.982 | 38.660 | 1.000 | 27.33 |
| ATOM | 1682 | CB  | GLN | A | 223 | 26.628 | -2.245 | 40.091 | 1.000 | 32.58 |
| ATOM | 1683 | CG  | GLN | A | 223 | 28.119 | -1.965 | 40.240 | 1.000 | 37.66 |
| ATOM | 1684 | CD  | GLN | A | 223 | 28.804 | -1.836 | 38.896 | 1.000 | 40.45 |
| ATOM | 1685 | OE1 | GLN | A | 223 | 28.765 | -2.759 | 38.076 | 1.000 | 70.90 |
| ATOM | 1686 | NE2 | GLN | A | 223 | 29.430 | -0.693 | 38.657 | 1.000 | 56.51 |
| ATOM | 1687 | C   | GLN | A | 223 | 24.952 | -2.916 | 38.387 | 1.000 | 25.59 |
| ATOM | 1688 | O   | GLN | A | 223 | 25.071 | -3.940 | 37.712 | 1.000 | 26.61 |
| ATOM | 1689 | N   | PHE | A | 224 | 23.794 | -2.560 | 38.945 | 1.000 | 23.53 |
| ATOM | 1690 | CA  | PHE | A | 224 | 22.586 | -3.328 | 38.637 | 1.000 | 26.71 |
| ATOM | 1691 | CB  | PHE | A | 224 | 21.408 | -2.714 | 39.374 | 1.000 | 23.63 |
| ATOM | 1692 | CG  | PHE | A | 224 | 20.093 | -3.429 | 39.226 | 1.000 | 23.65 |
| ATOM | 1693 | CD1 | PHE | A | 224 | 19.892 | -4.676 | 39.789 | 1.000 | 26.30 |
| ATOM | 1694 | CE1 | PHE | A | 224 | 18.688 | -5.341 | 39.670 | 1.000 | 23.27 |
| ATOM | 1695 | CZ  | PHE | A | 224 | 17.660 | -4.747 | 38.963 | 1.000 | 22.78 |
| ATOM | 1696 | CE2 | PHE | A | 224 | 17.843 | -3.504 | 38.397 | 1.000 | 21.02 |
| ATOM | 1697 | CD2 | PHE | A | 224 | 19.050 | -2.842 | 38.529 | 1.000 | 17.14 |
| ATOM | 1698 | C   | PHE | A | 224 | 22.335 | -3.340 | 37.135 | 1.000 | 29.21 |
| ATOM | 1699 | O   | PHE | A | 224 | 22.212 | -4.385 | 36.497 | 1.000 | 23.28 |
| ATOM | 1700 | N   | VAL | A | 225 | 22.272 | -2.147 | 36.539 | 1.000 | 29.45 |
| ATOM | 1701 | CA  | VAL | A | 225 | 22.003 | -2.057 | 35.103 | 1.000 | 23.17 |
| ATOM | 1702 | CB  | VAL | A | 225 | 22.017 | -0.597 | 34.616 | 1.000 | 27.27 |
| ATOM | 1703 | CG1 | VAL | A | 225 | 22.186 | -0.539 | 33.112 | 1.000 | 19.10 |
| ATOM | 1704 | CG2 | VAL | A | 225 | 20.732 | 0.108  | 35.045 | 1.000 | 33.43 |
| ATOM | 1705 | C   | VAL | A | 225 | 22.985 | -2.871 | 34.273 | 1.000 | 28.40 |
| ATOM | 1706 | O   | VAL | A | 225 | 22.554 | -3.638 | 33.400 | 1.000 | 25.05 |
| ATOM | 1707 | N   | ARG | A | 226 | 24.285 | -2.724 | 34.517 | 1.000 | 31.38 |
| ATOM | 1708 | CA  | ARG | A | 226 | 25.276 | -3.513 | 33.780 | 1.000 | 34.53 |
| ATOM | 1709 | CB  | ARG | A | 226 | 26.705 | -3.147 | 34.173 | 1.000 | 31.80 |
| ATOM | 1710 | CG  | ARG | A | 226 | 27.183 | -1.771 | 33.762 | 1.000 | 33.34 |
| ATOM | 1711 | CD  | ARG | A | 226 | 28.697 | -1.716 | 33.673 | 1.000 | 47.45 |
| ATOM | 1712 | NE  | ARG | A | 226 | 29.241 | -0.365 | 33.600 | 1.000 | 56.24 |
| ATOM | 1713 | CZ  | ARG | A | 226 | 29.961 | 0.232  | 34.542 | 1.000 | 62.79 |
| ATOM | 1714 | NH1 | ARG | A | 226 | 30.261 | -0.370 | 35.686 | 1.000 | 50.14 |
| ATOM | 1715 | NH2 | ARG | A | 226 | 30.401 | 1.471  | 34.354 | 1.000 | 74.65 |

**FIGURE 39**

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1716 | C   | ARG | A | 226 | 25.054 | -5.011  | 34.010 | 1.000 | 23.44 |
| ATOM | 1717 | O   | ARG | A | 226 | 25.301 | -5.826  | 33.118 | 1.000 | 30.89 |
| ATOM | 1718 | N   | THR | A | 227 | 24.582 | -5.377  | 35.195 | 1.000 | 21.86 |
| ATOM | 1719 | CA  | THR | A | 227 | 24.250 | -6.761  | 35.521 | 1.000 | 31.38 |
| ATOM | 1720 | CB  | THR | A | 227 | 23.825 | -6.921  | 36.994 | 1.000 | 37.64 |
| ATOM | 1721 | OG1 | THR | A | 227 | 24.903 | -6.608  | 37.874 | 1.000 | 34.53 |
| ATOM | 1722 | CG2 | THR | A | 227 | 23.457 | -8.365  | 37.306 | 1.000 | 22.45 |
| ATOM | 1723 | C   | THR | A | 227 | 23.108 | -7.250  | 34.627 | 1.000 | 32.76 |
| ATOM | 1724 | O   | THR | A | 227 | 23.237 | -8.240  | 33.912 | 1.000 | 27.21 |
| ATOM | 1725 | N   | VAL | A | 228 | 21.985 | -6.526  | 34.679 | 1.000 | 22.99 |
| ATOM | 1726 | CA  | VAL | A | 228 | 20.814 | -6.869  | 33.886 | 1.000 | 22.33 |
| ATOM | 1727 | CB  | VAL | A | 228 | 19.627 | -5.922  | 34.162 | 1.000 | 22.12 |
| ATOM | 1728 | CG1 | VAL | A | 228 | 18.466 | -6.213  | 33.221 | 1.000 | 17.66 |
| ATOM | 1729 | CG2 | VAL | A | 228 | 19.192 | -6.066  | 35.605 | 1.000 | 18.46 |
| ATOM | 1730 | C   | VAL | A | 228 | 21.140 | -6.859  | 32.397 | 1.000 | 21.49 |
| ATOM | 1731 | O   | VAL | A | 228 | 20.766 | -7.790  | 31.686 | 1.000 | 22.44 |
| ATOM | 1732 | N   | ARG | A | 229 | 21.821 | -5.824  | 31.914 | 1.000 | 19.91 |
| ATOM | 1733 | CA  | ARG | A | 229 | 22.183 | -5.792  | 30.489 | 1.000 | 30.48 |
| ATOM | 1734 | CB  | ARG | A | 229 | 22.877 | -4.480  | 30.149 | 1.000 | 30.12 |
| ATOM | 1735 | CG  | ARG | A | 229 | 23.502 | -4.301  | 28.786 | 1.000 | 28.02 |
| ATOM | 1736 | CD  | ARG | A | 229 | 22.590 | -4.596  | 27.614 | 1.000 | 26.85 |
| ATOM | 1737 | NE  | ARG | A | 229 | 21.290 | -3.951  | 27.719 | 1.000 | 26.70 |
| ATOM | 1738 | CZ  | ARG | A | 229 | 20.267 | -4.199  | 26.913 | 1.000 | 27.29 |
| ATOM | 1739 | NH1 | ARG | A | 229 | 20.394 | -5.079  | 25.930 | 1.000 | 20.12 |
| ATOM | 1740 | NH2 | ARG | A | 229 | 19.110 | -3.573  | 27.076 | 1.000 | 22.84 |
| ATOM | 1741 | C   | ARG | A | 229 | 23.041 | -7.010  | 30.156 | 1.000 | 42.31 |
| ATOM | 1742 | O   | ARG | A | 229 | 22.988 | -7.552  | 29.053 | 1.000 | 34.86 |
| ATOM | 1743 | N   | ASP | A | 230 | 23.842 | -7.483  | 31.114 | 1.000 | 40.71 |
| ATOM | 1744 | CA  | ASP | A | 230 | 24.637 | -8.682  | 30.882 | 1.000 | 32.09 |
| ATOM | 1745 | CB  | ASP | A | 230 | 25.480 | -9.003  | 32.118 | 1.000 | 31.74 |
| ATOM | 1746 | CG  | ASP | A | 230 | 26.543 | -10.044 | 31.824 | 1.000 | 48.14 |
| ATOM | 1747 | OD1 | ASP | A | 230 | 27.577 | -10.046 | 32.528 | 1.000 | 73.82 |
| ATOM | 1748 | OD2 | ASP | A | 230 | 26.357 | -10.865 | 30.899 | 1.000 | 48.16 |
| ATOM | 1749 | C   | ASP | A | 230 | 23.761 | -9.882  | 30.547 | 1.000 | 32.41 |
| ATOM | 1750 | O   | ASP | A | 230 | 24.000 | -10.629 | 29.598 | 1.000 | 36.42 |
| ATOM | 1751 | N   | TYR | A | 231 | 22.720 | -10.093 | 31.342 | 1.000 | 24.93 |
| ATOM | 1752 | CA  | TYR | A | 231 | 21.802 | -11.200 | 31.103 | 1.000 | 24.73 |
| ATOM | 1753 | CB  | TYR | A | 231 | 20.899 | -11.375 | 32.314 | 1.000 | 25.55 |
| ATOM | 1754 | CG  | TYR | A | 231 | 21.532 | -12.058 | 33.498 | 1.000 | 21.52 |
| ATOM | 1755 | CD1 | TYR | A | 231 | 22.248 | -11.325 | 34.429 | 1.000 | 20.07 |
| ATOM | 1756 | CE1 | TYR | A | 231 | 22.826 | -11.956 | 35.516 | 1.000 | 25.25 |
| ATOM | 1757 | CZ  | TYR | A | 231 | 22.690 | -13.315 | 35.684 | 1.000 | 23.69 |
| ATOM | 1758 | OH  | TYR | A | 231 | 23.272 | -13.934 | 36.770 | 1.000 | 36.60 |
| ATOM | 1759 | CE2 | TYR | A | 231 | 21.981 | -14.060 | 34.765 | 1.000 | 22.85 |
| ATOM | 1760 | CD2 | TYR | A | 231 | 21.406 | -13.431 | 33.678 | 1.000 | 23.77 |
| ATOM | 1761 | C   | TYR | A | 231 | 20.940 | -10.997 | 29.866 | 1.000 | 24.62 |
| ATOM | 1762 | O   | TYR | A | 231 | 20.658 | -11.948 | 29.137 | 1.000 | 34.40 |
| ATOM | 1763 | N   | ILE | A | 232 | 20.502 | -9.768  | 29.602 | 1.000 | 26.34 |
| ATOM | 1764 | CA  | ILE | A | 232 | 19.713 | -9.542  | 28.388 | 1.000 | 29.59 |
| ATOM | 1765 | CB  | ILE | A | 232 | 19.309 | -8.068  | 28.191 | 1.000 | 19.99 |
| ATOM | 1766 | CG1 | ILE | A | 232 | 18.283 | -7.551  | 29.204 | 1.000 | 21.05 |
| ATOM | 1767 | CD1 | ILE | A | 232 | 18.300 | -6.047  | 29.371 | 1.000 | 26.31 |

**FIGURE 40**

|      |      |     |     |   |     |        |         |        |       |       |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|-------|
| ATOM | 1768 | CG2 | ILE | A | 232 | 18.811 | -7.833  | 26.772 | 1.000 | 16.63 |
| ATOM | 1769 | C   | ILE | A | 232 | 20.497 | -9.985  | 27.153 | 1.000 | 25.92 |
| ATOM | 1770 | O   | ILE | A | 232 | 19.982 | -10.719 | 26.311 | 1.000 | 22.41 |
| ATOM | 1771 | N   | ASN | A | 233 | 21.741 | -9.526  | 27.075 | 1.000 | 21.03 |
| ATOM | 1772 | CA  | ASN | A | 233 | 22.573 | -9.788  | 25.900 | 1.000 | 32.05 |
| ATOM | 1773 | CB  | ASN | A | 233 | 23.931 | -9.102  | 26.027 | 1.000 | 31.19 |
| ATOM | 1774 | CG  | ASN | A | 233 | 23.891 | -7.603  | 25.830 | 1.000 | 35.15 |
| ATOM | 1775 | OD1 | ASN | A | 233 | 22.990 | -7.064  | 25.190 | 1.000 | 42.73 |
| ATOM | 1776 | ND2 | ASN | A | 233 | 24.873 | -6.892  | 26.379 | 1.000 | 33.97 |
| ATOM | 1777 | C   | ASN | A | 233 | 22.757 | -11.289 | 25.690 | 1.000 | 36.07 |
| ATOM | 1778 | O   | ASN | A | 233 | 22.998 | -11.738 | 24.575 | 1.000 | 43.18 |
| ATOM | 1779 | N   | ARG | A | 234 | 22.637 | -12.049 | 26.765 | 1.000 | 37.01 |
| ATOM | 1780 | CA  | ARG | A | 234 | 22.702 | -13.496 | 26.771 | 1.000 | 31.16 |
| ATOM | 1781 | CB  | ARG | A | 234 | 23.407 | -13.992 | 28.046 | 1.000 | 30.18 |
| ATOM | 1782 | CG  | ARG | A | 234 | 24.757 | -13.308 | 28.235 | 1.000 | 40.73 |
| ATOM | 1783 | CD  | ARG | A | 234 | 25.514 | -13.886 | 29.429 | 1.000 | 52.07 |
| ATOM | 1784 | NE  | ARG | A | 234 | 26.704 | -13.084 | 29.729 | 1.000 | 58.87 |
| ATOM | 1785 | CZ  | ARG | A | 234 | 27.879 | -13.610 | 30.055 | 1.000 | 65.29 |
| ATOM | 1786 | NH1 | ARG | A | 234 | 28.006 | -14.931 | 30.122 | 1.000 | 53.28 |
| ATOM | 1787 | NH2 | ARG | A | 234 | 28.913 | -12.818 | 30.313 | 1.000 | 60.98 |
| ATOM | 1788 | C   | ARG | A | 234 | 21.320 | -14.122 | 26.695 | 1.000 | 30.94 |
| ATOM | 1789 | O   | ARG | A | 234 | 21.130 | -15.307 | 26.977 | 1.000 | 24.57 |
| ATOM | 1790 | N   | SER | A | 235 | 20.307 | -13.346 | 26.303 | 1.000 | 26.15 |
| ATOM | 1791 | CA  | SER | A | 235 | 18.990 | -13.971 | 26.162 | 1.000 | 23.60 |
| ATOM | 1792 | CB  | SER | A | 235 | 17.959 | -13.293 | 27.058 | 1.000 | 26.05 |
| ATOM | 1793 | OG  | SER | A | 235 | 18.357 | -13.227 | 28.416 | 1.000 | 33.56 |
| ATOM | 1794 | C   | SER | A | 235 | 18.533 | -13.913 | 24.704 | 1.000 | 32.45 |
| ATOM | 1795 | O   | SER | A | 235 | 17.616 | -13.135 | 24.420 | 1.000 | 33.61 |
| ATOM | 1796 | N   | PRO | A | 236 | 19.136 | -14.685 | 23.805 | 1.000 | 44.30 |
| ATOM | 1797 | CA  | PRO | A | 236 | 18.740 | -14.662 | 22.393 | 1.000 | 39.17 |
| ATOM | 1798 | CB  | PRO | A | 236 | 19.695 | -15.646 | 21.714 | 1.000 | 48.74 |
| ATOM | 1799 | CG  | PRO | A | 236 | 20.068 | -16.584 | 22.822 | 1.000 | 52.35 |
| ATOM | 1800 | CD  | PRO | A | 236 | 20.220 | -15.667 | 24.009 | 1.000 | 52.02 |
| ATOM | 1801 | C   | PRO | A | 236 | 17.312 | -15.175 | 22.233 | 1.000 | 29.65 |
| ATOM | 1802 | O   | PRO | A | 236 | 16.908 | -16.104 | 22.941 | 1.000 | 30.54 |
| ATOM | 1803 | N   | GLY | A | 237 | 16.590 | -14.544 | 21.309 | 1.000 | 24.46 |
| ATOM | 1804 | CA  | GLY | A | 237 | 15.214 | -14.952 | 21.050 | 1.000 | 25.34 |
| ATOM | 1805 | C   | GLY | A | 237 | 14.233 | -14.388 | 22.054 | 1.000 | 26.14 |
| ATOM | 1806 | O   | GLY | A | 237 | 13.035 | -14.623 | 21.905 | 1.000 | 33.46 |
| ATOM | 1807 | N   | ALA | A | 238 | 14.681 | -13.642 | 23.069 | 1.000 | 22.93 |
| ATOM | 1808 | CA  | ALA | A | 238 | 13.739 | -13.094 | 24.042 | 1.000 | 17.40 |
| ATOM | 1809 | CB  | ALA | A | 238 | 14.491 | -12.542 | 25.253 | 1.000 | 20.22 |
| ATOM | 1810 | C   | ALA | A | 238 | 12.860 | -11.987 | 23.485 | 1.000 | 22.13 |
| ATOM | 1811 | O   | ALA | A | 238 | 13.305 | -11.162 | 22.683 | 1.000 | 22.14 |
| ATOM | 1812 | N   | GLY | A | 239 | 11.599 | -11.944 | 23.922 | 1.000 | 22.60 |
| ATOM | 1813 | CA  | GLY | A | 239 | 10.794 | -10.755 | 23.654 | 1.000 | 19.77 |
| ATOM | 1814 | C   | GLY | A | 239 | 11.314 | -9.578  | 24.475 | 1.000 | 23.04 |
| ATOM | 1815 | O   | GLY | A | 239 | 12.456 | -9.584  | 24.931 | 1.000 | 22.08 |
| ATOM | 1816 | N   | PRO | A | 240 | 10.501 | -8.544  | 24.664 | 1.000 | 20.46 |
| ATOM | 1817 | CA  | PRO | A | 240 | 10.904 | -7.365  | 25.418 | 1.000 | 18.32 |
| ATOM | 1818 | CB  | PRO | A | 240 | 9.645  | -6.478  | 25.441 | 1.000 | 15.24 |
| ATOM | 1819 | CG  | PRO | A | 240 | 8.855  | -6.953  | 24.270 | 1.000 | 26.50 |

**FIGURE 41**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1820 | CD  | PRO | A | 240 | 9.123  | -8.425 | 24.156 | 1.000 | 18.86 |
| ATOM | 1821 | C   | PRO | A | 240 | 11.261 | -7.689 | 26.866 | 1.000 | 24.79 |
| ATOM | 1822 | O   | PRO | A | 240 | 10.775 | -8.644 | 27.466 | 1.000 | 18.83 |
| ATOM | 1823 | N   | THR | A | 241 | 12.130 | -6.846 | 27.414 | 1.000 | 24.76 |
| ATOM | 1824 | CA  | THR | A | 241 | 12.452 | -6.849 | 28.822 | 1.000 | 19.34 |
| ATOM | 1825 | CB  | THR | A | 241 | 13.790 | -6.140 | 29.127 | 1.000 | 24.33 |
| ATOM | 1826 | OG1 | THR | A | 241 | 14.851 | -6.786 | 28.430 | 1.000 | 21.31 |
| ATOM | 1827 | CG2 | THR | A | 241 | 14.100 | -6.254 | 30.618 | 1.000 | 17.13 |
| ATOM | 1828 | C   | THR | A | 241 | 11.352 | -6.124 | 29.598 | 1.000 | 19.74 |
| ATOM | 1829 | O   | THR | A | 241 | 11.073 | -4.964 | 29.314 | 1.000 | 18.65 |
| ATOM | 1830 | N   | VAL | A | 242 | 10.731 | -6.769 | 30.576 | 1.000 | 19.16 |
| ATOM | 1831 | CA  | VAL | A | 242 | 9.738  | -6.070 | 31.381 | 1.000 | 24.84 |
| ATOM | 1832 | CB  | VAL | A | 242 | 8.698  | -7.016 | 32.012 | 1.000 | 25.33 |
| ATOM | 1833 | CG1 | VAL | A | 242 | 7.903  | -6.283 | 33.087 | 1.000 | 13.96 |
| ATOM | 1834 | CG2 | VAL | A | 242 | 7.778  | -7.573 | 30.936 | 1.000 | 18.53 |
| ATOM | 1835 | C   | VAL | A | 242 | 10.420 | -5.311 | 32.515 | 1.000 | 22.81 |
| ATOM | 1836 | O   | VAL | A | 242 | 11.202 | -5.907 | 33.245 | 1.000 | 15.62 |
| ATOM | 1837 | N   | VAL | A | 243 | 10.114 | -4.032 | 32.656 | 1.000 | 16.25 |
| ATOM | 1838 | CA  | VAL | A | 243 | 10.607 | -3.200 | 33.733 | 1.000 | 14.93 |
| ATOM | 1839 | CB  | VAL | A | 243 | 11.507 | -2.058 | 33.233 | 1.000 | 19.66 |
| ATOM | 1840 | CG1 | VAL | A | 243 | 12.145 | -1.357 | 34.424 | 1.000 | 17.79 |
| ATOM | 1841 | CG2 | VAL | A | 243 | 12.551 | -2.600 | 32.271 | 1.000 | 16.83 |
| ATOM | 1842 | C   | VAL | A | 243 | 9.437  | -2.590 | 34.489 | 1.000 | 18.40 |
| ATOM | 1843 | O   | VAL | A | 243 | 8.522  | -2.079 | 33.856 | 1.000 | 17.50 |
| ATOM | 1844 | N   | HIS | A | 244 | 9.469  | -2.655 | 35.821 | 1.000 | 14.50 |
| ATOM | 1845 | CA  | HIS | A | 244 | 8.388  | -2.005 | 36.543 | 1.000 | 19.33 |
| ATOM | 1846 | CB  | HIS | A | 244 | 7.200  | -2.952 | 36.704 | 1.000 | 15.76 |
| ATOM | 1847 | CG  | HIS | A | 244 | 7.362  | -4.005 | 37.749 | 1.000 | 15.99 |
| ATOM | 1848 | ND1 | HIS | A | 244 | 7.060  | -3.783 | 39.076 | 1.000 | 16.28 |
| ATOM | 1849 | CE1 | HIS | A | 244 | 7.293  | -4.893 | 39.761 | 1.000 | 23.84 |
| ATOM | 1850 | NE2 | HIS | A | 244 | 7.736  | -5.820 | 38.934 | 1.000 | 18.37 |
| ATOM | 1851 | CD2 | HIS | A | 244 | 7.785  | -5.289 | 37.665 | 1.000 | 12.59 |
| ATOM | 1852 | C   | HIS | A | 244 | 8.868  | -1.514 | 37.906 | 1.000 | 22.68 |
| ATOM | 1853 | O   | HIS | A | 244 | 9.879  | -1.996 | 38.398 | 1.000 | 22.27 |
| ATOM | 1854 | N   | CYS | A | 245 | 8.127  | -0.563 | 38.448 | 1.000 | 22.48 |
| ATOM | 1855 | CA  | CYS | A | 245 | 8.229  | -0.136 | 39.836 | 1.000 | 22.65 |
| ATOM | 1856 | CB  | CYS | A | 245 | 8.861  | 1.241  | 39.990 | 1.000 | 16.47 |
| ATOM | 1857 | SG  | CYS | A | 245 | 8.219  | 2.535  | 38.895 | 1.000 | 26.22 |
| ATOM | 1858 | C   | CYS | A | 245 | 6.812  | -0.194 | 40.402 | 1.000 | 23.88 |
| ATOM | 1859 | O   | CYS | A | 245 | 6.094  | -1.173 | 40.153 | 1.000 | 26.38 |
| ATOM | 1860 | N   | SER | A | 246 | 6.385  | 0.833  | 41.132 | 1.000 | 17.80 |
| ATOM | 1861 | CA  | SER | A | 246 | 4.995  | 0.806  | 41.607 | 1.000 | 11.67 |
| ATOM | 1862 | CB  | SER | A | 246 | 4.853  | 1.726  | 42.821 | 1.000 | 26.78 |
| ATOM | 1863 | OG  | SER | A | 246 | 3.561  | 1.643  | 43.393 | 1.000 | 30.47 |
| ATOM | 1864 | C   | SER | A | 246 | 4.033  | 1.208  | 40.501 | 1.000 | 11.21 |
| ATOM | 1865 | O   | SER | A | 246 | 3.068  | 0.510  | 40.185 | 1.000 | 20.25 |
| ATOM | 1866 | N   | ALA | A | 247 | 4.286  | 2.377  | 39.909 | 1.000 | 15.30 |
| ATOM | 1867 | CA  | ALA | A | 247 | 3.455  | 2.947  | 38.871 | 1.000 | 13.07 |
| ATOM | 1868 | CB  | ALA | A | 247 | 3.302  | 4.446  | 39.102 | 1.000 | 23.22 |
| ATOM | 1869 | C   | ALA | A | 247 | 4.008  | 2.710  | 37.468 | 1.000 | 17.09 |
| ATOM | 1870 | O   | ALA | A | 247 | 3.286  | 2.806  | 36.473 | 1.000 | 23.76 |
| ATOM | 1871 | N   | GLY | A | 248 | 5.300  | 2.413  | 37.353 | 1.000 | 15.64 |

FIGURE 42

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |        |        |       |       |
|------|------|-----|-----------|--------|--------|--------|-------|-------|
| ATOM | 1872 | CA  | GLY A 248 | 5.920  | 2.177  | 36.056 | 1.000 | 19.79 |
| ATOM | 1873 | C   | GLY A 248 | 6.329  | 3.497  | 35.413 | 1.000 | 28.08 |
| ATOM | 1874 | O   | GLY A 248 | 6.206  | 3.654  | 34.200 | 1.000 | 29.60 |
| ATOM | 1875 | N   | VAL A 249 | 6.828  | 4.410  | 36.242 | 1.000 | 24.91 |
| ATOM | 1876 | CA  | VAL A 249 | 7.165  | 5.771  | 35.893 | 1.000 | 28.97 |
| ATOM | 1877 | CB  | VAL A 249 | 6.349  | 6.742  | 36.799 | 1.000 | 36.67 |
| ATOM | 1878 | CG1 | VAL A 249 | 4.984  | 6.994  | 36.192 | 1.000 | 26.78 |
| ATOM | 1879 | CG2 | VAL A 249 | 6.223  | 6.201  | 38.219 | 1.000 | 28.45 |
| ATOM | 1880 | C   | VAL A 249 | 8.635  | 6.167  | 36.035 | 1.000 | 29.09 |
| ATOM | 1881 | O   | VAL A 249 | 9.456  | 5.930  | 35.151 | 1.000 | 32.80 |
| ATOM | 1882 | N   | GLY A 250 | 8.941  | 6.823  | 37.144 | 1.000 | 24.19 |
| ATOM | 1883 | CA  | GLY A 250 | 10.149 | 7.515  | 37.501 | 1.000 | 19.59 |
| ATOM | 1884 | C   | GLY A 250 | 11.344 | 6.573  | 37.577 | 1.000 | 14.84 |
| ATOM | 1885 | O   | GLY A 250 | 12.267 | 6.702  | 36.763 | 1.000 | 27.35 |
| ATOM | 1886 | N   | ARG A 251 | 11.280 | 5.662  | 38.534 | 1.000 | 11.74 |
| ATOM | 1887 | CA  | ARG A 251 | 12.347 | 4.688  | 38.735 | 1.000 | 15.59 |
| ATOM | 1888 | CB  | ARG A 251 | 12.096 | 3.823  | 39.969 | 1.000 | 21.64 |
| ATOM | 1889 | CG  | ARG A 251 | 11.869 | 4.624  | 41.250 | 1.000 | 23.80 |
| ATOM | 1890 | CD  | ARG A 251 | 11.653 | 3.670  | 42.416 | 1.000 | 23.58 |
| ATOM | 1891 | NE  | ARG A 251 | 11.390 | 4.352  | 43.679 | 1.000 | 22.88 |
| ATOM | 1892 | CZ  | ARG A 251 | 11.100 | 3.675  | 44.791 | 1.000 | 22.64 |
| ATOM | 1893 | NH1 | ARG A 251 | 11.042 | 2.354  | 44.756 | 1.000 | 26.67 |
| ATOM | 1894 | NH2 | ARG A 251 | 10.865 | 4.301  | 45.931 | 1.000 | 21.50 |
| ATOM | 1895 | C   | ARG A 251 | 12.517 | 3.790  | 37.513 | 1.000 | 19.15 |
| ATOM | 1896 | O   | ARG A 251 | 13.649 | 3.477  | 37.144 | 1.000 | 23.13 |
| ATOM | 1897 | N   | THR A 252 | 11.409 | 3.372  | 36.904 | 1.000 | 18.67 |
| ATOM | 1898 | CA  | THR A 252 | 11.482 | 2.546  | 35.702 | 1.000 | 18.13 |
| ATOM | 1899 | CB  | THR A 252 | 10.103 | 2.014  | 35.289 | 1.000 | 20.50 |
| ATOM | 1900 | OG1 | THR A 252 | 9.706  | 1.005  | 36.228 | 1.000 | 22.47 |
| ATOM | 1901 | CG2 | THR A 252 | 10.127 | 1.333  | 33.924 | 1.000 | 18.43 |
| ATOM | 1902 | C   | THR A 252 | 12.101 | 3.351  | 34.562 | 1.000 | 20.66 |
| ATOM | 1903 | O   | THR A 252 | 13.001 | 2.852  | 33.877 | 1.000 | 22.41 |
| ATOM | 1904 | N   | GLY A 253 | 11.627 | 4.580  | 34.377 | 1.000 | 19.06 |
| ATOM | 1905 | CA  | GLY A 253 | 12.124 | 5.407  | 33.276 | 1.000 | 24.03 |
| ATOM | 1906 | C   | GLY A 253 | 13.615 | 5.663  | 33.423 | 1.000 | 26.29 |
| ATOM | 1907 | O   | GLY A 253 | 14.370 | 5.727  | 32.452 | 1.000 | 20.33 |
| ATOM | 1908 | N   | THR A 254 | 14.036 | 5.811  | 34.674 | 1.000 | 20.94 |
| ATOM | 1909 | CA  | THR A 254 | 15.433 | 6.059  | 35.011 | 1.000 | 25.32 |
| ATOM | 1910 | CB  | THR A 254 | 15.546 | 6.439  | 36.505 | 1.000 | 23.28 |
| ATOM | 1911 | OG1 | THR A 254 | 14.879 | 7.688  | 36.704 | 1.000 | 19.41 |
| ATOM | 1912 | CG2 | THR A 254 | 16.993 | 6.642  | 36.910 | 1.000 | 22.36 |
| ATOM | 1913 | C   | THR A 254 | 16.300 | 4.847  | 34.714 | 1.000 | 22.06 |
| ATOM | 1914 | O   | THR A 254 | 17.389 | 4.928  | 34.151 | 1.000 | 27.89 |
| ATOM | 1915 | N   | PHE A 255 | 15.811 | 3.671  | 35.094 | 1.000 | 18.65 |
| ATOM | 1916 | CA  | PHE A 255 | 16.498 | 2.433  | 34.780 | 1.000 | 13.27 |
| ATOM | 1917 | CB  | PHE A 255 | 15.709 | 1.219  | 35.277 | 1.000 | 13.04 |
| ATOM | 1918 | CG  | PHE A 255 | 16.305 | -0.125 | 34.923 | 1.000 | 21.43 |
| ATOM | 1919 | CD1 | PHE A 255 | 17.222 | -0.717 | 35.783 | 1.000 | 22.29 |
| ATOM | 1920 | CE1 | PHE A 255 | 17.786 | -1.941 | 35.492 | 1.000 | 24.82 |
| ATOM | 1921 | CZ  | PHE A 255 | 17.476 | -2.615 | 34.325 | 1.000 | 20.78 |
| ATOM | 1922 | CE2 | PHE A 255 | 16.558 | -2.054 | 33.461 | 1.000 | 16.57 |
| ATOM | 1923 | CD2 | PHE A 255 | 15.987 | -0.836 | 33.778 | 1.000 | 20.56 |

**FIGURE 43**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1924 | C   | PHE | A | 255 | 16.721 | 2.323  | 33.277 | 1.000 | 23.91 |
| ATOM | 1925 | O   | PHE | A | 255 | 17.791 | 1.918  | 32.814 | 1.000 | 23.04 |
| ATOM | 1926 | N   | ILE | A | 256 | 15.665 | 2.620  | 32.511 | 1.000 | 21.98 |
| ATOM | 1927 | CA  | ILE | A | 256 | 15.794 | 2.334  | 31.082 | 1.000 | 23.48 |
| ATOM | 1928 | CB  | ILE | A | 256 | 14.462 | 2.211  | 30.336 | 1.000 | 22.01 |
| ATOM | 1929 | CG1 | ILE | A | 256 | 13.667 | 0.941  | 30.657 | 1.000 | 26.28 |
| ATOM | 1930 | CD1 | ILE | A | 256 | 12.210 | 1.020  | 30.221 | 1.000 | 23.52 |
| ATOM | 1931 | CG2 | ILE | A | 256 | 14.666 | 2.310  | 28.823 | 1.000 | 17.05 |
| ATOM | 1932 | C   | ILE | A | 256 | 16.666 | 3.412  | 30.439 | 1.000 | 14.97 |
| ATOM | 1933 | O   | ILE | A | 256 | 17.470 | 3.058  | 29.575 | 1.000 | 20.35 |
| ATOM | 1934 | N   | ALA | A | 257 | 16.489 | 4.659  | 30.864 | 1.000 | 16.95 |
| ATOM | 1935 | CA  | ALA | A | 257 | 17.365 | 5.725  | 30.354 | 1.000 | 13.62 |
| ATOM | 1936 | CB  | ALA | A | 257 | 16.973 | 7.077  | 30.894 | 1.000 | 16.03 |
| ATOM | 1937 | C   | ALA | A | 257 | 18.811 | 5.373  | 30.689 | 1.000 | 20.04 |
| ATOM | 1938 | O   | ALA | A | 257 | 19.713 | 5.497  | 29.866 | 1.000 | 24.71 |
| ATOM | 1939 | N   | LEU | A | 258 | 19.083 | 4.886  | 31.908 | 1.000 | 20.59 |
| ATOM | 1940 | CA  | LEU | A | 258 | 20.490 | 4.560  | 32.186 | 1.000 | 25.52 |
| ATOM | 1941 | CB  | LEU | A | 258 | 20.723 | 4.299  | 33.673 | 1.000 | 29.22 |
| ATOM | 1942 | CG  | LEU | A | 258 | 22.171 | 4.177  | 34.151 | 1.000 | 33.36 |
| ATOM | 1943 | CD1 | LEU | A | 258 | 23.069 | 5.186  | 33.453 | 1.000 | 17.44 |
| ATOM | 1944 | CD2 | LEU | A | 258 | 22.268 | 4.363  | 35.660 | 1.000 | 32.48 |
| ATOM | 1945 | C   | LEU | A | 258 | 20.931 | 3.377  | 31.336 | 1.000 | 24.80 |
| ATOM | 1946 | O   | LEU | A | 258 | 22.020 | 3.447  | 30.768 | 1.000 | 31.87 |
| ATOM | 1947 | N   | ASP | A | 259 | 20.130 | 2.316  | 31.238 | 1.000 | 19.82 |
| ATOM | 1948 | CA  | ASP | A | 259 | 20.524 | 1.155  | 30.439 | 1.000 | 21.21 |
| ATOM | 1949 | CB  | ASP | A | 259 | 19.441 | 0.080  | 30.461 | 1.000 | 26.62 |
| ATOM | 1950 | CG  | ASP | A | 259 | 19.716 | -1.155 | 29.637 | 1.000 | 33.72 |
| ATOM | 1951 | OD1 | ASP | A | 259 | 20.883 | -1.598 | 29.573 | 1.000 | 35.74 |
| ATOM | 1952 | OD2 | ASP | A | 259 | 18.758 | -1.719 | 29.046 | 1.000 | 24.80 |
| ATOM | 1953 | C   | ASP | A | 259 | 20.832 | 1.579  | 29.010 | 1.000 | 21.68 |
| ATOM | 1954 | O   | ASP | A | 259 | 21.742 | 1.052  | 28.372 | 1.000 | 28.89 |
| ATOM | 1955 | N   | ARG | A | 260 | 20.070 | 2.539  | 28.506 | 1.000 | 23.42 |
| ATOM | 1956 | CA  | ARG | A | 260 | 20.230 | 3.024  | 27.138 | 1.000 | 25.06 |
| ATOM | 1957 | CB  | ARG | A | 260 | 19.028 | 3.897  | 26.771 | 1.000 | 28.71 |
| ATOM | 1958 | CG  | ARG | A | 260 | 17.920 | 3.218  | 25.983 | 1.000 | 37.83 |
| ATOM | 1959 | CD  | ARG | A | 260 | 17.815 | 3.892  | 24.612 | 1.000 | 40.41 |
| ATOM | 1960 | NE  | ARG | A | 260 | 16.447 | 4.236  | 24.289 | 1.000 | 39.10 |
| ATOM | 1961 | CZ  | ARG | A | 260 | 15.997 | 5.081  | 23.376 | 1.000 | 37.92 |
| ATOM | 1962 | NH1 | ARG | A | 260 | 16.820 | 5.759  | 22.595 | 1.000 | 44.18 |
| ATOM | 1963 | NH2 | ARG | A | 260 | 14.682 | 5.235  | 23.257 | 1.000 | 38.91 |
| ATOM | 1964 | C   | ARG | A | 260 | 21.503 | 3.834  | 26.932 | 1.000 | 28.89 |
| ATOM | 1965 | O   | ARG | A | 260 | 22.183 | 3.707  | 25.913 | 1.000 | 28.43 |
| ATOM | 1966 | N   | ILE | A | 261 | 21.850 | 4.713  | 27.878 | 1.000 | 31.24 |
| ATOM | 1967 | CA  | ILE | A | 261 | 23.011 | 5.568  | 27.644 | 1.000 | 32.00 |
| ATOM | 1968 | CB  | ILE | A | 261 | 23.003 | 6.871  | 28.463 | 1.000 | 30.49 |
| ATOM | 1969 | CG1 | ILE | A | 261 | 23.174 | 6.692  | 29.969 | 1.000 | 33.74 |
| ATOM | 1970 | CD1 | ILE | A | 261 | 22.668 | 7.864  | 30.782 | 1.000 | 47.87 |
| ATOM | 1971 | CG2 | ILE | A | 261 | 21.747 | 7.669  | 28.142 | 1.000 | 38.62 |
| ATOM | 1972 | C   | ILE | A | 261 | 24.311 | 4.827  | 27.939 | 1.000 | 30.43 |
| ATOM | 1973 | O   | ILE | A | 261 | 25.293 | 5.061  | 27.228 | 1.000 | 33.25 |
| ATOM | 1974 | N   | LEU | A | 262 | 24.317 | 3.958  | 28.951 | 1.000 | 22.89 |
| ATOM | 1975 | CA  | LEU | A | 262 | 25.541 | 3.189  | 29.202 | 1.000 | 27.21 |

**FIGURE 44**



|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1976 | CB  | LEU | A | 262 | 25.411 | 2.219  | 30.368 | 1.000 | 29.63 |
| ATOM | 1977 | CG  | LEU | A | 262 | 25.330 | 2.760  | 31.793 | 1.000 | 38.46 |
| ATOM | 1978 | CD1 | LEU | A | 262 | 25.371 | 1.630  | 32.815 | 1.000 | 28.64 |
| ATOM | 1979 | CD2 | LEU | A | 262 | 26.441 | 3.762  | 32.059 | 1.000 | 34.63 |
| ATOM | 1980 | C   | LEU | A | 262 | 25.912 | 2.424  | 27.931 | 1.000 | 37.42 |
| ATOM | 1981 | O   | LEU | A | 262 | 27.090 | 2.228  | 27.640 | 1.000 | 48.70 |
| ATOM | 1982 | N   | GLN | A | 263 | 24.900 | 1.987  | 27.183 | 1.000 | 40.24 |
| ATOM | 1983 | CA  | GLN | A | 263 | 25.151 | 1.267  | 25.943 | 1.000 | 38.78 |
| ATOM | 1984 | CB  | GLN | A | 263 | 23.875 | 0.706  | 25.322 | 1.000 | 30.36 |
| ATOM | 1985 | CG  | GLN | A | 263 | 23.653 | -0.767 | 25.637 | 1.000 | 26.81 |
| ATOM | 1986 | CD  | GLN | A | 263 | 22.223 | -1.212 | 25.423 | 1.000 | 28.10 |
| ATOM | 1987 | OE1 | GLN | A | 263 | 21.946 | -1.976 | 24.500 | 1.000 | 30.64 |
| ATOM | 1988 | NE2 | GLN | A | 263 | 21.304 | -0.760 | 26.273 | 1.000 | 33.75 |
| ATOM | 1989 | C   | GLN | A | 263 | 25.827 | 2.190  | 24.934 | 1.000 | 44.56 |
| ATOM | 1990 | O   | GLN | A | 263 | 26.667 | 1.744  | 24.161 | 1.000 | 46.96 |
| ATOM | 1991 | N   | GLN | A | 264 | 25.420 | 3.455  | 24.977 | 1.000 | 42.51 |
| ATOM | 1992 | CA  | GLN | A | 264 | 25.954 | 4.431  | 24.033 | 1.000 | 47.48 |
| ATOM | 1993 | CB  | GLN | A | 264 | 25.220 | 5.773  | 24.152 | 1.000 | 39.34 |
| ATOM | 1994 | CG  | GLN | A | 264 | 23.957 | 5.807  | 23.303 | 1.000 | 37.99 |
| ATOM | 1995 | CD  | GLN | A | 264 | 23.060 | 6.989  | 23.591 | 1.000 | 42.10 |
| ATOM | 1996 | OE1 | GLN | A | 264 | 23.477 | 7.972  | 24.206 | 1.000 | 41.41 |
| ATOM | 1997 | NE2 | GLN | A | 264 | 21.814 | 6.899  | 23.144 | 1.000 | 49.45 |
| ATOM | 1998 | C   | GLN | A | 264 | 27.452 | 4.610  | 24.256 | 1.000 | 50.33 |
| ATOM | 1999 | O   | GLN | A | 264 | 28.253 | 4.493  | 23.328 | 1.000 | 38.61 |
| ATOM | 2000 | N   | LEU | A | 265 | 27.777 | 4.876  | 25.513 | 1.000 | 49.87 |
| ATOM | 2001 | CA  | LEU | A | 265 | 29.118 | 5.176  | 25.984 | 1.000 | 51.23 |
| ATOM | 2002 | CB  | LEU | A | 265 | 29.084 | 5.389  | 27.503 | 1.000 | 48.71 |
| ATOM | 2003 | CG  | LEU | A | 265 | 28.256 | 6.584  | 27.988 | 1.000 | 49.68 |
| ATOM | 2004 | CD1 | LEU | A | 265 | 28.263 | 6.684  | 29.507 | 1.000 | 46.47 |
| ATOM | 2005 | CD2 | LEU | A | 265 | 28.757 | 7.884  | 27.370 | 1.000 | 44.07 |
| ATOM | 2006 | C   | LEU | A | 265 | 30.122 | 4.097  | 25.607 | 1.000 | 59.08 |
| ATOM | 2007 | O   | LEU | A | 265 | 31.329 | 4.351  | 25.565 | 1.000 | 62.01 |
| ATOM | 2008 | N   | ASP | A | 266 | 29.656 | 2.887  | 25.317 | 1.000 | 60.11 |
| ATOM | 2009 | CA  | ASP | A | 266 | 30.559 | 1.815  | 24.901 | 1.000 | 60.82 |
| ATOM | 2010 | CB  | ASP | A | 266 | 30.345 | 0.581  | 25.776 | 1.000 | 68.15 |
| ATOM | 2011 | CG  | ASP | A | 266 | 30.603 | 0.832  | 27.251 | 1.000 | 74.94 |
| ATOM | 2012 | OD1 | ASP | A | 266 | 31.286 | 1.822  | 27.599 | 1.000 | 87.47 |
| ATOM | 2013 | OD2 | ASP | A | 266 | 30.117 | 0.033  | 28.083 | 1.000 | 72.82 |
| ATOM | 2014 | C   | ASP | A | 266 | 30.362 | 1.481  | 23.428 | 1.000 | 56.29 |
| ATOM | 2015 | O   | ASP | A | 266 | 30.797 | 0.449  | 22.918 | 1.000 | 65.03 |
| ATOM | 2016 | N   | SER | A | 267 | 29.692 | 2.373  | 22.703 | 1.000 | 49.36 |
| ATOM | 2017 | CA  | SER | A | 267 | 29.450 | 2.133  | 21.286 | 1.000 | 49.97 |
| ATOM | 2018 | CB  | SER | A | 267 | 28.040 | 1.563  | 21.092 | 1.000 | 47.54 |
| ATOM | 2019 | OG  | SER | A | 267 | 28.070 | 0.147  | 21.070 | 1.000 | 70.07 |
| ATOM | 2020 | C   | SER | A | 267 | 29.602 | 3.403  | 20.457 | 1.000 | 56.45 |
| ATOM | 2021 | O   | SER | A | 267 | 29.833 | 3.345  | 19.249 | 1.000 | 64.11 |
| ATOM | 2022 | N   | LYS | A | 268 | 29.457 | 4.547  | 21.113 | 1.000 | 54.03 |
| ATOM | 2023 | CA  | LYS | A | 268 | 29.450 | 5.851  | 20.473 | 1.000 | 61.77 |
| ATOM | 2024 | CB  | LYS | A | 268 | 28.124 | 6.565  | 20.747 | 1.000 | 73.01 |
| ATOM | 2025 | CG  | LYS | A | 268 | 27.792 | 7.746  | 19.856 | 1.000 | 78.98 |
| ATOM | 2026 | CD  | LYS | A | 268 | 26.344 | 7.687  | 19.384 | 1.000 | 85.20 |
| ATOM | 2027 | CE  | LYS | A | 268 | 25.589 | 8.983  | 19.679 | 1.000 | 87.23 |

FIGURE 45

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2028 | NZ  | LYS | A | 268 | 24.372 | 8.773  | 20.503 | 1.000 | 77.94 |
| ATOM | 2029 | C   | LYS | A | 268 | 30.607 | 6.721  | 20.967 | 1.000 | 57.67 |
| ATOM | 2030 | O   | LYS | A | 268 | 31.288 | 6.352  | 21.923 | 1.000 | 56.55 |
| ATOM | 2031 | N   | ASP | A | 269 | 30.759 | 7.842  | 20.289 | 1.000 | 51.51 |
| ATOM | 2032 | CA  | ASP | A | 269 | 31.664 | 8.925  | 20.619 | 1.000 | 61.39 |
| ATOM | 2033 | CB  | ASP | A | 269 | 32.424 | 9.415  | 19.388 | 1.000 | 66.41 |
| ATOM | 2034 | CG  | ASP | A | 269 | 31.625 | 9.286  | 18.106 | 1.000 | 74.35 |
| ATOM | 2035 | OD1 | ASP | A | 269 | 32.119 | 8.629  | 17.162 | 1.000 | 91.04 |
| ATOM | 2036 | OD2 | ASP | A | 269 | 30.505 | 9.842  | 18.044 | 1.000 | 81.62 |
| ATOM | 2037 | C   | ASP | A | 269 | 30.865 | 10.067 | 21.240 | 1.000 | 58.72 |
| ATOM | 2038 | O   | ASP | A | 269 | 31.369 | 11.104 | 21.659 | 1.000 | 48.76 |
| ATOM | 2039 | N   | SER | A | 270 | 29.551 | 9.848  | 21.289 | 1.000 | 55.39 |
| ATOM | 2040 | CA  | SER | A | 270 | 28.687 | 10.847 | 21.910 | 1.000 | 53.30 |
| ATOM | 2041 | CB  | SER | A | 270 | 27.989 | 11.679 | 20.834 | 1.000 | 46.93 |
| ATOM | 2042 | OG  | SER | A | 270 | 27.692 | 10.829 | 19.734 | 1.000 | 51.09 |
| ATOM | 2043 | C   | SER | A | 270 | 27.674 | 10.148 | 22.807 | 1.000 | 54.77 |
| ATOM | 2044 | O   | SER | A | 270 | 27.500 | 8.934  | 22.703 | 1.000 | 57.87 |
| ATOM | 2045 | N   | VAL | A | 271 | 27.031 | 10.915 | 23.668 | 1.000 | 51.16 |
| ATOM | 2046 | CA  | VAL | A | 271 | 26.025 | 10.400 | 24.590 | 1.000 | 47.16 |
| ATOM | 2047 | CB  | VAL | A | 271 | 26.612 | 10.189 | 25.992 | 1.000 | 43.33 |
| ATOM | 2048 | CG1 | VAL | A | 271 | 27.075 | 11.525 | 26.564 | 1.000 | 28.98 |
| ATOM | 2049 | CG2 | VAL | A | 271 | 25.609 | 9.523  | 26.918 | 1.000 | 33.32 |
| ATOM | 2050 | C   | VAL | A | 271 | 24.851 | 11.374 | 24.626 | 1.000 | 51.02 |
| ATOM | 2051 | O   | VAL | A | 271 | 25.054 | 12.585 | 24.754 | 1.000 | 45.80 |
| ATOM | 2052 | N   | ASP | A | 272 | 23.639 | 10.841 | 24.484 | 1.000 | 43.19 |
| ATOM | 2053 | CA  | ASP | A | 272 | 22.451 | 11.680 | 24.350 | 1.000 | 34.67 |
| ATOM | 2054 | CB  | ASP | A | 272 | 21.819 | 11.492 | 22.973 | 1.000 | 34.66 |
| ATOM | 2055 | CG  | ASP | A | 272 | 20.791 | 12.553 | 22.633 | 1.000 | 34.78 |
| ATOM | 2056 | OD1 | ASP | A | 272 | 20.496 | 13.413 | 23.488 | 1.000 | 35.05 |
| ATOM | 2057 | OD2 | ASP | A | 272 | 20.262 | 12.537 | 21.499 | 1.000 | 61.92 |
| ATOM | 2058 | C   | ASP | A | 272 | 21.450 | 11.367 | 25.450 | 1.000 | 37.86 |
| ATOM | 2059 | O   | ASP | A | 272 | 20.601 | 10.489 | 25.312 | 1.000 | 33.07 |
| ATOM | 2060 | N   | ILE | A | 273 | 21.548 | 12.095 | 26.564 | 1.000 | 29.66 |
| ATOM | 2061 | CA  | ILE | A | 273 | 20.651 | 11.774 | 27.671 | 1.000 | 30.56 |
| ATOM | 2062 | CB  | ILE | A | 273 | 21.245 | 12.212 | 29.019 | 1.000 | 28.78 |
| ATOM | 2063 | CG1 | ILE | A | 273 | 22.562 | 11.518 | 29.362 | 1.000 | 24.46 |
| ATOM | 2064 | CD1 | ILE | A | 273 | 23.227 | 12.049 | 30.612 | 1.000 | 33.99 |
| ATOM | 2065 | CG2 | ILE | A | 273 | 20.228 | 12.016 | 30.134 | 1.000 | 24.56 |
| ATOM | 2066 | C   | ILE | A | 273 | 19.290 | 12.420 | 27.450 | 1.000 | 36.66 |
| ATOM | 2067 | O   | ILE | A | 273 | 18.264 | 11.844 | 27.813 | 1.000 | 38.74 |
| ATOM | 2068 | N   | TYR | A | 274 | 19.301 | 13.608 | 26.845 | 1.000 | 31.39 |
| ATOM | 2069 | CA  | TYR | A | 274 | 18.044 | 14.276 | 26.525 | 1.000 | 27.62 |
| ATOM | 2070 | CB  | TYR | A | 274 | 18.312 | 15.642 | 25.908 | 1.000 | 26.54 |
| ATOM | 2071 | CG  | TYR | A | 274 | 17.119 | 16.489 | 25.551 | 1.000 | 27.58 |
| ATOM | 2072 | CD1 | TYR | A | 274 | 16.633 | 17.434 | 26.450 | 1.000 | 29.05 |
| ATOM | 2073 | CE1 | TYR | A | 274 | 15.544 | 18.225 | 26.150 | 1.000 | 28.10 |
| ATOM | 2074 | CZ  | TYR | A | 274 | 14.913 | 18.089 | 24.932 | 1.000 | 28.89 |
| ATOM | 2075 | OH  | TYR | A | 274 | 13.827 | 18.881 | 24.631 | 1.000 | 40.18 |
| ATOM | 2076 | CE2 | TYR | A | 274 | 15.372 | 17.169 | 24.020 | 1.000 | 30.70 |
| ATOM | 2077 | CD2 | TYR | A | 274 | 16.469 | 16.377 | 24.331 | 1.000 | 31.75 |
| ATOM | 2078 | C   | TYR | A | 274 | 17.228 | 13.415 | 25.565 | 1.000 | 30.07 |
| ATOM | 2079 | O   | TYR | A | 274 | 16.027 | 13.221 | 25.735 | 1.000 | 27.79 |

**FIGURE 46**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2080 | N   | GLY | A | 275 | 17.908 | 12.908 | 24.540 | 1.000 | 30.84 |
| ATOM | 2081 | CA  | GLY | A | 275 | 17.256 | 12.132 | 23.499 | 1.000 | 38.31 |
| ATOM | 2082 | C   | GLY | A | 275 | 16.611 | 10.863 | 24.016 | 1.000 | 36.93 |
| ATOM | 2083 | O   | GLY | A | 275 | 15.515 | 10.487 | 23.605 | 1.000 | 33.21 |
| ATOM | 2084 | N   | ALA | A | 276 | 17.282 | 10.176 | 24.930 | 1.000 | 26.01 |
| ATOM | 2085 | CA  | ALA | A | 276 | 16.728 | 8.949  | 25.490 | 1.000 | 26.10 |
| ATOM | 2086 | CB  | ALA | A | 276 | 17.753 | 8.300  | 26.409 | 1.000 | 36.77 |
| ATOM | 2087 | C   | ALA | A | 276 | 15.440 | 9.236  | 26.248 | 1.000 | 26.60 |
| ATOM | 2088 | O   | ALA | A | 276 | 14.412 | 8.600  | 26.061 | 1.000 | 21.84 |
| ATOM | 2089 | N   | VAL | A | 277 | 15.510 | 10.227 | 27.129 | 1.000 | 27.46 |
| ATOM | 2090 | CA  | VAL | A | 277 | 14.382 | 10.602 | 27.971 | 1.000 | 26.38 |
| ATOM | 2091 | CB  | VAL | A | 277 | 14.829 | 11.656 | 29.004 | 1.000 | 27.97 |
| ATOM | 2092 | CG1 | VAL | A | 277 | 13.661 | 12.343 | 29.687 | 1.000 | 33.02 |
| ATOM | 2093 | CG2 | VAL | A | 277 | 15.720 | 10.980 | 30.043 | 1.000 | 17.52 |
| ATOM | 2094 | C   | VAL | A | 277 | 13.229 | 11.103 | 27.113 | 1.000 | 26.05 |
| ATOM | 2095 | O   | VAL | A | 277 | 12.060 | 10.837 | 27.417 | 1.000 | 29.47 |
| ATOM | 2096 | N   | HIS | A | 278 | 13.556 | 11.815 | 26.043 | 1.000 | 20.60 |
| ATOM | 2097 | CA  | HIS | A | 278 | 12.558 | 12.336 | 25.113 | 1.000 | 25.33 |
| ATOM | 2098 | CB  | HIS | A | 278 | 13.204 | 13.259 | 24.087 | 1.000 | 27.86 |
| ATOM | 2099 | CG  | HIS | A | 278 | 12.276 | 13.815 | 23.054 | 1.000 | 25.27 |
| ATOM | 2100 | ND1 | HIS | A | 278 | 11.807 | 13.069 | 21.994 | 1.000 | 24.22 |
| ATOM | 2101 | CE1 | HIS | A | 278 | 11.015 | 13.819 | 21.244 | 1.000 | 24.97 |
| ATOM | 2102 | NE2 | HIS | A | 278 | 10.961 | 15.031 | 21.773 | 1.000 | 23.92 |
| ATOM | 2103 | CD2 | HIS | A | 278 | 11.746 | 15.050 | 22.900 | 1.000 | 22.15 |
| ATOM | 2104 | C   | HIS | A | 278 | 11.838 | 11.214 | 24.370 | 1.000 | 23.01 |
| ATOM | 2105 | O   | HIS | A | 278 | 10.650 | 11.288 | 24.068 | 1.000 | 25.09 |
| ATOM | 2106 | N   | ASP | A | 279 | 12.571 | 10.160 | 24.059 | 1.000 | 20.73 |
| ATOM | 2107 | CA  | ASP | A | 279 | 11.994 | 9.026  | 23.343 | 1.000 | 24.89 |
| ATOM | 2108 | CB  | ASP | A | 279 | 13.099 | 8.159  | 22.746 | 1.000 | 30.17 |
| ATOM | 2109 | CG  | ASP | A | 279 | 12.727 | 7.306  | 21.558 | 1.000 | 30.34 |
| ATOM | 2110 | OD1 | ASP | A | 279 | 12.077 | 7.787  | 20.605 | 1.000 | 26.50 |
| ATOM | 2111 | OD2 | ASP | A | 279 | 13.096 | 6.106  | 21.539 | 1.000 | 33.56 |
| ATOM | 2112 | C   | ASP | A | 279 | 11.131 | 8.228  | 24.309 | 1.000 | 19.27 |
| ATOM | 2113 | O   | ASP | A | 279 | 10.059 | 7.720  | 23.981 | 1.000 | 23.16 |
| ATOM | 2114 | N   | LEU | A | 280 | 11.627 | 8.121  | 25.541 | 1.000 | 17.51 |
| ATOM | 2115 | CA  | LEU | A | 280 | 10.848 | 7.371  | 26.523 | 1.000 | 25.22 |
| ATOM | 2116 | CB  | LEU | A | 280 | 11.578 | 7.273  | 27.857 | 1.000 | 22.56 |
| ATOM | 2117 | CG  | LEU | A | 280 | 12.948 | 6.595  | 27.878 | 1.000 | 30.97 |
| ATOM | 2118 | CD1 | LEU | A | 280 | 13.309 | 6.169  | 29.294 | 1.000 | 16.61 |
| ATOM | 2119 | CD2 | LEU | A | 280 | 12.998 | 5.407  | 26.930 | 1.000 | 39.44 |
| ATOM | 2120 | C   | LEU | A | 280 | 9.475  | 8.027  | 26.702 | 1.000 | 28.43 |
| ATOM | 2121 | O   | LEU | A | 280 | 8.472  | 7.315  | 26.678 | 1.000 | 19.82 |
| ATOM | 2122 | N   | ARG | A | 281 | 9.480  | 9.335  | 26.877 | 1.000 | 27.78 |
| ATOM | 2123 | CA  | ARG | A | 281 | 8.364  | 10.230 | 27.097 | 1.000 | 26.26 |
| ATOM | 2124 | CB  | ARG | A | 281 | 8.840  | 11.690 | 27.129 | 1.000 | 27.59 |
| ATOM | 2125 | CG  | ARG | A | 281 | 9.597  | 12.025 | 28.413 | 1.000 | 35.06 |
| ATOM | 2126 | CD  | ARG | A | 281 | 8.645  | 11.966 | 29.597 | 1.000 | 33.64 |
| ATOM | 2127 | NE  | ARG | A | 281 | 9.295  | 12.376 | 30.831 | 1.000 | 36.75 |
| ATOM | 2128 | CZ  | ARG | A | 281 | 9.526  | 13.626 | 31.204 | 1.000 | 40.89 |
| ATOM | 2129 | NH1 | ARG | A | 281 | 9.161  | 14.636 | 30.435 | 1.000 | 32.39 |
| ATOM | 2130 | NH2 | ARG | A | 281 | 10.132 | 13.874 | 32.361 | 1.000 | 61.48 |
| ATOM | 2131 | C   | ARG | A | 281 | 7.302  | 10.096 | 26.018 | 1.000 | 19.40 |

**FIGURE 47**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |       |        |        |       |       |
|------|------|-----|-----|---|-----|-------|--------|--------|-------|-------|
| ATOM | 2132 | O   | ARG | A | 281 | 6.104 | 10.236 | 26.254 | 1.000 | 20.20 |
| ATOM | 2133 | N   | LEU | A | 282 | 7.773 | 9.823  | 24.805 | 1.000 | 20.07 |
| ATOM | 2134 | CA  | LEU | A | 282 | 6.823 | 9.651  | 23.711 | 1.000 | 23.11 |
| ATOM | 2135 | CB  | LEU | A | 282 | 7.523 | 9.589  | 22.353 | 1.000 | 17.59 |
| ATOM | 2136 | CG  | LEU | A | 282 | 7.893 | 10.913 | 21.688 | 1.000 | 27.09 |
| ATOM | 2137 | CD1 | LEU | A | 282 | 8.800 | 10.679 | 20.489 | 1.000 | 27.56 |
| ATOM | 2138 | CD2 | LEU | A | 282 | 6.660 | 11.688 | 21.243 | 1.000 | 20.11 |
| ATOM | 2139 | C   | LEU | A | 282 | 5.974 | 8.404  | 23.913 | 1.000 | 26.60 |
| ATOM | 2140 | O   | LEU | A | 282 | 4.880 | 8.342  | 23.352 | 1.000 | 22.78 |
| ATOM | 2141 | N   | HIS | A | 283 | 6.430 | 7.412  | 24.678 | 1.000 | 25.41 |
| ATOM | 2142 | CA  | HIS | A | 283 | 5.698 | 6.144  | 24.667 | 1.000 | 19.57 |
| ATOM | 2143 | CB  | HIS | A | 283 | 6.688 | 5.008  | 24.336 | 1.000 | 24.33 |
| ATOM | 2144 | CG  | HIS | A | 283 | 7.263 | 5.215  | 22.965 | 1.000 | 22.62 |
| ATOM | 2145 | ND1 | HIS | A | 283 | 6.742 | 4.619  | 21.841 | 1.000 | 26.42 |
| ATOM | 2146 | CE1 | HIS | A | 283 | 7.436 | 4.985  | 20.775 | 1.000 | 25.06 |
| ATOM | 2147 | NE2 | HIS | A | 283 | 8.386 | 5.808  | 21.174 | 1.000 | 24.57 |
| ATOM | 2148 | CD2 | HIS | A | 283 | 8.300 | 5.974  | 22.536 | 1.000 | 21.10 |
| ATOM | 2149 | C   | HIS | A | 283 | 4.956 | 5.861  | 25.961 | 1.000 | 17.31 |
| ATOM | 2150 | O   | HIS | A | 283 | 4.101 | 4.976  | 26.006 | 1.000 | 20.69 |
| ATOM | 2151 | N   | ARG | A | 284 | 5.262 | 6.606  | 27.011 | 1.000 | 16.92 |
| ATOM | 2152 | CA  | ARG | A | 284 | 4.594 | 6.512  | 28.296 | 1.000 | 15.56 |
| ATOM | 2153 | CB  | ARG | A | 284 | 5.038 | 5.279  | 29.091 | 1.000 | 19.52 |
| ATOM | 2154 | CG  | ARG | A | 284 | 4.214 | 5.010  | 30.355 | 1.000 | 16.19 |
| ATOM | 2155 | CD  | ARG | A | 284 | 4.569 | 3.660  | 30.954 | 1.000 | 19.69 |
| ATOM | 2156 | NE  | ARG | A | 284 | 4.009 | 3.428  | 32.282 | 1.000 | 18.76 |
| ATOM | 2157 | CZ  | ARG | A | 284 | 2.892 | 2.731  | 32.492 | 1.000 | 19.76 |
| ATOM | 2158 | NH1 | ARG | A | 284 | 2.214 | 2.207  | 31.475 | 1.000 | 11.48 |
| ATOM | 2159 | NH2 | ARG | A | 284 | 2.439 | 2.553  | 33.726 | 1.000 | 17.29 |
| ATOM | 2160 | C   | ARG | A | 284 | 4.845 | 7.774  | 29.119 | 1.000 | 15.30 |
| ATOM | 2161 | O   | ARG | A | 284 | 5.941 | 8.327  | 29.076 | 1.000 | 25.00 |
| ATOM | 2162 | N   | VAL | A | 285 | 3.834 | 8.221  | 29.846 | 1.000 | 19.78 |
| ATOM | 2163 | CA  | VAL | A | 285 | 3.912 | 9.415  | 30.685 | 1.000 | 26.66 |
| ATOM | 2164 | CB  | VAL | A | 285 | 2.507 | 9.771  | 31.215 | 1.000 | 32.12 |
| ATOM | 2165 | CG1 | VAL | A | 285 | 1.981 | 8.686  | 32.152 | 1.000 | 20.70 |
| ATOM | 2166 | CG2 | VAL | A | 285 | 2.503 | 11.126 | 31.909 | 1.000 | 29.12 |
| ATOM | 2167 | C   | VAL | A | 285 | 4.917 | 9.216  | 31.814 | 1.000 | 20.03 |
| ATOM | 2168 | O   | VAL | A | 285 | 5.153 | 8.085  | 32.242 | 1.000 | 23.27 |
| ATOM | 2169 | N   | HIS | A | 286 | 5.510 | 10.296 | 32.281 | 1.000 | 28.92 |
| ATOM | 2170 | CA  | HIS | A | 286 | 6.440 | 10.404 | 33.382 | 1.000 | 29.32 |
| ATOM | 2171 | CB  | HIS | A | 286 | 5.744 | 10.052 | 34.718 | 1.000 | 33.92 |
| ATOM | 2172 | CG  | HIS | A | 286 | 4.476 | 10.821 | 34.904 | 1.000 | 38.90 |
| ATOM | 2173 | ND1 | HIS | A | 286 | 4.430 | 12.188 | 34.769 | 1.000 | 45.43 |
| ATOM | 2174 | CE1 | HIS | A | 286 | 3.197 | 12.615 | 34.978 | 1.000 | 45.72 |
| ATOM | 2175 | NE2 | HIS | A | 286 | 2.439 | 11.567 | 35.244 | 1.000 | 48.04 |
| ATOM | 2176 | CD2 | HIS | A | 286 | 3.216 | 10.433 | 35.200 | 1.000 | 47.11 |
| ATOM | 2177 | C   | HIS | A | 286 | 7.669 | 9.521  | 33.267 | 1.000 | 24.27 |
| ATOM | 2178 | O   | HIS | A | 286 | 8.292 | 9.259  | 34.303 | 1.000 | 39.87 |
| ATOM | 2179 | N   | MET | A | 287 | 8.054 | 9.038  | 32.087 | 1.000 | 19.82 |
| ATOM | 2180 | CA  | MET | A | 287 | 9.326 | 8.294  | 32.047 | 1.000 | 18.04 |
| ATOM | 2181 | CB  | MET | A | 287 | 9.579 | 7.694  | 30.679 | 1.000 | 19.24 |
| ATOM | 2182 | CG  | MET | A | 287 | 8.566 | 6.647  | 30.239 | 1.000 | 24.10 |
| ATOM | 2183 | SD  | MET | A | 287 | 8.699 | 5.134  | 31.234 | 1.000 | 32.12 |

**FIGURE 48**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2184 | CE  | MET | A | 287 | 7.526  | 5.570  | 32.521 | 1.000 | 32.04 |
| ATOM | 2185 | C   | MET | A | 287 | 10.457 | 9.247  | 32.459 | 1.000 | 32.08 |
| ATOM | 2186 | O   | MET | A | 287 | 10.732 | 10.211 | 31.741 | 1.000 | 32.41 |
| ATOM | 2187 | N   | VAL | A | 288 | 11.071 | 8.981  | 33.599 | 1.000 | 29.73 |
| ATOM | 2188 | CA  | VAL | A | 288 | 12.024 | 9.837  | 34.294 | 1.000 | 22.00 |
| ATOM | 2189 | CB  | VAL | A | 288 | 13.229 | 10.233 | 33.436 | 1.000 | 21.06 |
| ATOM | 2190 | CG1 | VAL | A | 288 | 14.167 | 11.132 | 34.232 | 1.000 | 28.71 |
| ATOM | 2191 | CG2 | VAL | A | 288 | 13.961 | 8.986  | 32.952 | 1.000 | 15.73 |
| ATOM | 2192 | C   | VAL | A | 288 | 11.269 | 11.073 | 34.787 | 1.000 | 30.61 |
| ATOM | 2193 | O   | VAL | A | 288 | 11.226 | 12.112 | 34.132 | 1.000 | 31.06 |
| ATOM | 2194 | N   | GLN | A | 289 | 10.675 | 10.871 | 35.957 | 1.000 | 23.90 |
| ATOM | 2195 | CA  | GLN | A | 289 | 9.626  | 11.709 | 36.494 | 1.000 | 28.48 |
| ATOM | 2196 | CB  | GLN | A | 289 | 8.735  | 10.869 | 37.427 | 1.000 | 27.94 |
| ATOM | 2197 | CG  | GLN | A | 289 | 7.406  | 11.535 | 37.748 | 1.000 | 34.50 |
| ATOM | 2198 | CD  | GLN | A | 289 | 6.481  | 10.661 | 38.562 | 1.000 | 30.01 |
| ATOM | 2199 | OE1 | GLN | A | 289 | 6.907  | 9.646  | 39.112 | 1.000 | 45.90 |
| ATOM | 2200 | NE2 | GLN | A | 289 | 5.209  | 11.026 | 38.655 | 1.000 | 37.56 |
| ATOM | 2201 | C   | GLN | A | 289 | 10.123 | 12.924 | 37.258 | 1.000 | 36.20 |
| ATOM | 2202 | O   | GLN | A | 289 | 9.316  | 13.811 | 37.536 | 1.000 | 32.67 |
| ATOM | 2203 | N   | THR | A | 290 | 11.402 | 12.994 | 37.619 | 1.000 | 33.43 |
| ATOM | 2204 | CA  | THR | A | 290 | 11.857 | 14.147 | 38.382 | 1.000 | 32.24 |
| ATOM | 2205 | CB  | THR | A | 290 | 12.078 | 13.862 | 39.878 | 1.000 | 27.63 |
| ATOM | 2206 | OG1 | THR | A | 290 | 13.285 | 13.106 | 40.043 | 1.000 | 42.04 |
| ATOM | 2207 | CG2 | THR | A | 290 | 10.951 | 13.021 | 40.456 | 1.000 | 35.76 |
| ATOM | 2208 | C   | THR | A | 290 | 13.174 | 14.677 | 37.822 | 1.000 | 42.79 |
| ATOM | 2209 | O   | THR | A | 290 | 13.921 | 13.935 | 37.191 | 1.000 | 31.85 |
| ATOM | 2210 | N   | GLU | A | 291 | 13.421 | 15.963 | 38.072 | 1.000 | 41.73 |
| ATOM | 2211 | CA  | GLU | A | 291 | 14.707 | 16.538 | 37.692 | 1.000 | 33.95 |
| ATOM | 2212 | CB  | GLU | A | 291 | 14.749 | 18.032 | 37.980 | 1.000 | 44.06 |
| ATOM | 2213 | CG  | GLU | A | 291 | 16.167 | 18.595 | 38.042 | 1.000 | 51.27 |
| ATOM | 2214 | CD  | GLU | A | 291 | 16.146 | 20.001 | 38.627 | 1.000 | 50.92 |
| ATOM | 2215 | OE1 | GLU | A | 291 | 16.994 | 20.298 | 39.487 | 1.000 | 46.66 |
| ATOM | 2216 | OE2 | GLU | A | 291 | 15.255 | 20.769 | 38.205 | 1.000 | 44.79 |
| ATOM | 2217 | C   | GLU | A | 291 | 15.814 | 15.826 | 38.461 | 1.000 | 26.05 |
| ATOM | 2218 | O   | GLU | A | 291 | 16.890 | 15.581 | 37.921 | 1.000 | 31.12 |
| ATOM | 2219 | N   | CYS | A | 292 | 15.513 | 15.486 | 39.714 | 1.000 | 27.69 |
| ATOM | 2220 | CA  | CYS | A | 292 | 16.460 | 14.750 | 40.550 | 1.000 | 22.15 |
| ATOM | 2221 | CB  | CYS | A | 292 | 15.840 | 14.409 | 41.899 | 1.000 | 28.25 |
| ATOM | 2222 | SG  | CYS | A | 292 | 16.996 | 13.623 | 43.050 | 1.000 | 68.90 |
| ATOM | 2223 | C   | CYS | A | 292 | 16.908 | 13.477 | 39.849 | 1.000 | 29.87 |
| ATOM | 2224 | O   | CYS | A | 292 | 18.079 | 13.092 | 39.819 | 1.000 | 32.69 |
| ATOM | 2225 | N   | GLN | A | 293 | 15.924 | 12.801 | 39.246 | 1.000 | 28.10 |
| ATOM | 2226 | CA  | GLN | A | 293 | 16.294 | 11.621 | 38.459 | 1.000 | 28.74 |
| ATOM | 2227 | CB  | GLN | A | 293 | 15.030 | 10.845 | 38.087 | 1.000 | 25.18 |
| ATOM | 2228 | CG  | GLN | A | 293 | 14.509 | 10.017 | 39.250 | 1.000 | 22.15 |
| ATOM | 2229 | CD  | GLN | A | 293 | 13.034 | 9.698  | 39.089 | 1.000 | 27.52 |
| ATOM | 2230 | OE1 | GLN | A | 293 | 12.412 | 10.175 | 38.141 | 1.000 | 28.92 |
| ATOM | 2231 | NE2 | GLN | A | 293 | 12.503 | 8.909  | 40.009 | 1.000 | 24.69 |
| ATOM | 2232 | C   | GLN | A | 293 | 17.097 | 12.037 | 37.235 | 1.000 | 29.57 |
| ATOM | 2233 | O   | GLN | A | 293 | 18.056 | 11.373 | 36.831 | 1.000 | 25.56 |
| ATOM | 2234 | N   | TYR | A | 294 | 16.706 | 13.165 | 36.640 | 1.000 | 27.49 |
| ATOM | 2235 | CA  | TYR | A | 294 | 17.399 | 13.690 | 35.469 | 1.000 | 28.60 |

**FIGURE 49**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2236 | CB  | TYR | A | 294 | 16.667 | 14.921 | 34.934 | 1.000 | 26.37 |
| ATOM | 2237 | CG  | TYR | A | 294 | 17.095 | 15.300 | 33.540 | 1.000 | 27.25 |
| ATOM | 2238 | CD1 | TYR | A | 294 | 16.934 | 14.379 | 32.509 | 1.000 | 37.08 |
| ATOM | 2239 | CE1 | TYR | A | 294 | 17.311 | 14.682 | 31.218 | 1.000 | 37.31 |
| ATOM | 2240 | CZ  | TYR | A | 294 | 17.861 | 15.920 | 30.951 | 1.000 | 39.27 |
| ATOM | 2241 | OH  | TYR | A | 294 | 18.234 | 16.214 | 29.659 | 1.000 | 43.06 |
| ATOM | 2242 | CE2 | TYR | A | 294 | 18.030 | 16.846 | 31.957 | 1.000 | 36.04 |
| ATOM | 2243 | CD2 | TYR | A | 294 | 17.648 | 16.535 | 33.252 | 1.000 | 28.82 |
| ATOM | 2244 | C   | TYR | A | 294 | 18.844 | 14.045 | 35.798 | 1.000 | 26.82 |
| ATOM | 2245 | O   | TYR | A | 294 | 19.783 | 13.828 | 35.040 | 1.000 | 34.04 |
| ATOM | 2246 | N   | VAL | A | 295 | 19.062 | 14.611 | 36.978 | 1.000 | 22.51 |
| ATOM | 2247 | CA  | VAL | A | 295 | 20.439 | 14.894 | 37.384 | 1.000 | 32.33 |
| ATOM | 2248 | CB  | VAL | A | 295 | 20.466 | 15.733 | 38.675 | 1.000 | 34.92 |
| ATOM | 2249 | CG1 | VAL | A | 295 | 21.858 | 15.698 | 39.282 | 1.000 | 36.74 |
| ATOM | 2250 | CG2 | VAL | A | 295 | 20.006 | 17.152 | 38.372 | 1.000 | 28.93 |
| ATOM | 2251 | C   | VAL | A | 295 | 21.228 | 13.612 | 37.608 | 1.000 | 27.09 |
| ATOM | 2252 | O   | VAL | A | 295 | 22.364 | 13.460 | 37.153 | 1.000 | 34.90 |
| ATOM | 2253 | N   | TYR | A | 296 | 20.606 | 12.678 | 38.319 | 1.000 | 26.27 |
| ATOM | 2254 | CA  | TYR | A | 296 | 21.232 | 11.378 | 38.578 | 1.000 | 29.32 |
| ATOM | 2255 | CB  | TYR | A | 296 | 20.229 | 10.492 | 39.314 | 1.000 | 28.67 |
| ATOM | 2256 | CG  | TYR | A | 296 | 20.761 | 9.196  | 39.861 | 1.000 | 35.66 |
| ATOM | 2257 | CD1 | TYR | A | 296 | 21.638 | 9.150  | 40.937 | 1.000 | 33.98 |
| ATOM | 2258 | CE1 | TYR | A | 296 | 22.119 | 7.951  | 41.431 | 1.000 | 32.73 |
| ATOM | 2259 | CZ  | TYR | A | 296 | 21.722 | 6.770  | 40.842 | 1.000 | 33.73 |
| ATOM | 2260 | OH  | TYR | A | 296 | 22.187 | 5.561  | 41.318 | 1.000 | 35.73 |
| ATOM | 2261 | CE2 | TYR | A | 296 | 20.853 | 6.786  | 39.775 | 1.000 | 33.85 |
| ATOM | 2262 | CD2 | TYR | A | 296 | 20.376 | 7.987  | 39.290 | 1.000 | 37.49 |
| ATOM | 2263 | C   | TYR | A | 296 | 21.742 | 10.739 | 37.295 | 1.000 | 27.66 |
| ATOM | 2264 | O   | TYR | A | 296 | 22.831 | 10.150 | 37.266 | 1.000 | 32.42 |
| ATOM | 2265 | N   | LEU | A | 297 | 21.015 | 10.840 | 36.184 | 1.000 | 26.94 |
| ATOM | 2266 | CA  | LEU | A | 297 | 21.497 | 10.174 | 34.968 | 1.000 | 28.80 |
| ATOM | 2267 | CB  | LEU | A | 297 | 20.459 | 10.187 | 33.846 | 1.000 | 24.99 |
| ATOM | 2268 | CG  | LEU | A | 297 | 19.141 | 9.462  | 34.135 | 1.000 | 24.86 |
| ATOM | 2269 | CD1 | LEU | A | 297 | 18.119 | 9.734  | 33.046 | 1.000 | 23.89 |
| ATOM | 2270 | CD2 | LEU | A | 297 | 19.357 | 7.966  | 34.270 | 1.000 | 20.37 |
| ATOM | 2271 | C   | LEU | A | 297 | 22.795 | 10.820 | 34.495 | 1.000 | 33.04 |
| ATOM | 2272 | O   | LEU | A | 297 | 23.704 | 10.129 | 34.036 | 1.000 | 49.72 |
| ATOM | 2273 | N   | HIS | A | 298 | 22.879 | 12.139 | 34.606 | 1.000 | 31.51 |
| ATOM | 2274 | CA  | HIS | A | 298 | 24.115 | 12.850 | 34.291 | 1.000 | 35.13 |
| ATOM | 2275 | CB  | HIS | A | 298 | 23.871 | 14.358 | 34.261 | 1.000 | 40.34 |
| ATOM | 2276 | CG  | HIS | A | 298 | 22.964 | 14.791 | 33.153 | 1.000 | 37.19 |
| ATOM | 2277 | ND1 | HIS | A | 298 | 21.598 | 14.646 | 33.222 | 1.000 | 31.89 |
| ATOM | 2278 | CE1 | HIS | A | 298 | 21.052 | 15.109 | 32.108 | 1.000 | 37.29 |
| ATOM | 2279 | NE2 | HIS | A | 298 | 22.021 | 15.545 | 31.322 | 1.000 | 38.18 |
| ATOM | 2280 | CD2 | HIS | A | 298 | 23.228 | 15.356 | 31.954 | 1.000 | 36.75 |
| ATOM | 2281 | C   | HIS | A | 298 | 25.202 | 12.524 | 35.310 | 1.000 | 29.73 |
| ATOM | 2282 | O   | HIS | A | 298 | 26.358 | 12.314 | 34.945 | 1.000 | 36.94 |
| ATOM | 2283 | N   | GLN | A | 299 | 24.848 | 12.470 | 36.599 | 1.000 | 26.95 |
| ATOM | 2284 | CA  | GLN | A | 299 | 25.880 | 12.104 | 37.579 | 1.000 | 34.87 |
| ATOM | 2285 | CB  | GLN | A | 299 | 25.339 | 12.184 | 39.001 | 1.000 | 34.33 |
| ATOM | 2286 | CG  | GLN | A | 299 | 24.925 | 13.584 | 39.424 | 1.000 | 44.04 |
| ATOM | 2287 | CD  | GLN | A | 299 | 24.110 | 13.598 | 40.702 | 1.000 | 49.76 |

FIGURE 50

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2288 | OE1 | GLN | A | 299 | 23.289 | 12.715 | 40.953 | 1.000 | 45.00 |
| ATOM | 2289 | NE2 | GLN | A | 299 | 24.315 | 14.612 | 41.540 | 1.000 | 34.03 |
| ATOM | 2290 | C   | GLN | A | 299 | 26.425 | 10.712 | 37.267 | 1.000 | 42.34 |
| ATOM | 2291 | O   | GLN | A | 299 | 27.602 | 10.424 | 37.494 | 1.000 | 36.30 |
| ATOM | 2292 | N   | CYS | A | 300 | 25.565 | 9.845  | 36.732 | 1.000 | 40.53 |
| ATOM | 2293 | CA  | CYS | A | 300 | 25.967 | 8.486  | 36.389 | 1.000 | 34.21 |
| ATOM | 2294 | CB  | CYS | A | 300 | 24.743 | 7.622  | 36.058 | 1.000 | 28.55 |
| ATOM | 2295 | SG  | CYS | A | 300 | 23.923 | 6.884  | 37.493 | 1.000 | 33.04 |
| ATOM | 2296 | C   | CYS | A | 300 | 26.937 | 8.476  | 35.217 | 1.000 | 34.71 |
| ATOM | 2297 | O   | CYS | A | 300 | 27.937 | 7.754  | 35.210 | 1.000 | 29.76 |
| ATOM | 2298 | N   | VAL | A | 301 | 26.651 | 9.279  | 34.193 | 1.000 | 43.45 |
| ATOM | 2299 | CA  | VAL | A | 301 | 27.534 | 9.265  | 33.021 | 1.000 | 48.01 |
| ATOM | 2300 | CB  | VAL | A | 301 | 26.875 | 9.944  | 31.809 | 1.000 | 44.81 |
| ATOM | 2301 | CG1 | VAL | A | 301 | 27.860 | 10.046 | 30.650 | 1.000 | 34.28 |
| ATOM | 2302 | CG2 | VAL | A | 301 | 25.626 | 9.187  | 31.372 | 1.000 | 34.53 |
| ATOM | 2303 | C   | VAL | A | 301 | 28.865 | 9.935  | 33.351 | 1.000 | 51.69 |
| ATOM | 2304 | O   | VAL | A | 301 | 29.937 | 9.511  | 32.918 | 1.000 | 43.92 |
| ATOM | 2305 | N   | ARG | A | 302 | 28.808 | 11.008 | 34.140 | 1.000 | 49.27 |
| ATOM | 2306 | CA  | ARG | A | 302 | 30.013 | 11.730 | 34.519 | 1.000 | 45.50 |
| ATOM | 2307 | CB  | ARG | A | 302 | 29.670 | 12.984 | 35.328 | 1.000 | 43.11 |
| ATOM | 2308 | CG  | ARG | A | 302 | 30.898 | 13.642 | 35.952 | 1.000 | 44.65 |
| ATOM | 2309 | CD  | ARG | A | 302 | 30.517 | 14.426 | 37.200 | 1.000 | 42.63 |
| ATOM | 2310 | NE  | ARG | A | 302 | 30.239 | 13.510 | 38.308 | 1.000 | 45.99 |
| ATOM | 2311 | CZ  | ARG | A | 302 | 29.458 | 13.803 | 39.336 | 1.000 | 50.62 |
| ATOM | 2312 | NH1 | ARG | A | 302 | 28.871 | 14.992 | 39.398 | 1.000 | 51.05 |
| ATOM | 2313 | NH2 | ARG | A | 302 | 29.264 | 12.909 | 40.297 | 1.000 | 48.05 |
| ATOM | 2314 | C   | ARG | A | 302 | 30.955 | 10.852 | 35.332 | 1.000 | 44.54 |
| ATOM | 2315 | O   | ARG | A | 302 | 32.162 | 10.831 | 35.095 | 1.000 | 56.02 |
| ATOM | 2316 | N   | ASP | A | 303 | 30.409 | 10.124 | 36.305 | 1.000 | 44.54 |
| ATOM | 2317 | CA  | ASP | A | 303 | 31.292 | 9.270  | 37.105 | 1.000 | 43.81 |
| ATOM | 2318 | CB  | ASP | A | 303 | 30.542 | 8.705  | 38.312 | 1.000 | 34.49 |
| ATOM | 2319 | CG  | ASP | A | 303 | 30.053 | 9.823  | 39.215 | 1.000 | 37.57 |
| ATOM | 2320 | OD1 | ASP | A | 303 | 30.540 | 10.963 | 39.057 | 1.000 | 52.86 |
| ATOM | 2321 | OD2 | ASP | A | 303 | 29.183 | 9.594  | 40.078 | 1.000 | 46.64 |
| ATOM | 2322 | C   | ASP | A | 303 | 31.889 | 8.163  | 36.248 | 1.000 | 48.14 |
| ATOM | 2323 | O   | ASP | A | 303 | 33.015 | 7.724  | 36.489 | 1.000 | 65.82 |
| ATOM | 2324 | N   | VAL | A | 304 | 31.151 | 7.703  | 35.241 | 1.000 | 50.71 |
| ATOM | 2325 | CA  | VAL | A | 304 | 31.668 | 6.631  | 34.389 | 1.000 | 49.88 |
| ATOM | 2326 | CB  | VAL | A | 304 | 30.541 | 5.917  | 33.628 | 1.000 | 51.23 |
| ATOM | 2327 | CG1 | VAL | A | 304 | 30.871 | 5.761  | 32.150 | 1.000 | 50.73 |
| ATOM | 2328 | CG2 | VAL | A | 304 | 30.277 | 4.561  | 34.263 | 1.000 | 34.30 |
| ATOM | 2329 | C   | VAL | A | 304 | 32.697 | 7.175  | 33.404 | 1.000 | 41.63 |
| ATOM | 2330 | O   | VAL | A | 304 | 33.656 | 6.498  | 33.037 | 1.000 | 41.23 |
| ATOM | 2331 | N   | LEU | A | 305 | 32.489 | 8.413  | 32.981 | 1.000 | 46.33 |
| ATOM | 2332 | CA  | LEU | A | 305 | 33.442 | 9.091  | 32.106 | 1.000 | 57.09 |
| ATOM | 2333 | CB  | LEU | A | 305 | 32.783 | 10.338 | 31.507 | 1.000 | 52.07 |
| ATOM | 2334 | CG  | LEU | A | 305 | 31.872 | 10.008 | 30.314 | 1.000 | 47.93 |
| ATOM | 2335 | CD1 | LEU | A | 305 | 31.630 | 11.216 | 29.427 | 1.000 | 48.09 |
| ATOM | 2336 | CD2 | LEU | A | 305 | 32.488 | 8.860  | 29.529 | 1.000 | 30.69 |
| ATOM | 2337 | C   | LEU | A | 305 | 34.728 | 9.439  | 32.849 | 1.000 | 64.87 |
| ATOM | 2338 | O   | LEU | A | 305 | 35.814 | 9.387  | 32.266 | 1.000 | 58.87 |
| ATOM | 2339 | N   | ARG | A | 306 | 34.601 | 9.776  | 34.127 | 1.000 | 68.65 |

FIGURE 51

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |        |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|--------|
| ATOM | 2340 | CA  | ARG | A | 306 | 35.714 | 10.014 | 35.032 | 1.000 | 66.90  |
| ATOM | 2341 | CB  | ARG | A | 306 | 35.210 | 10.407 | 36.420 | 1.000 | 62.97  |
| ATOM | 2342 | CG  | ARG | A | 306 | 34.909 | 11.889 | 36.584 | 1.000 | 63.46  |
| ATOM | 2343 | CD  | ARG | A | 306 | 34.233 | 12.132 | 37.927 | 1.000 | 63.67  |
| ATOM | 2344 | NE  | ARG | A | 306 | 33.867 | 13.537 | 38.091 | 1.000 | 72.26  |
| ATOM | 2345 | CZ  | ARG | A | 306 | 33.178 | 13.982 | 39.131 | 1.000 | 81.44  |
| ATOM | 2346 | NH1 | ARG | A | 306 | 32.786 | 13.132 | 40.074 | 1.000 | 88.77  |
| ATOM | 2347 | NH2 | ARG | A | 306 | 32.874 | 15.266 | 39.234 | 1.000 | 94.65  |
| ATOM | 2348 | C   | ARG | A | 306 | 36.601 | 8.773  | 35.157 | 1.000 | 69.05  |
| ATOM | 2349 | O   | ARG | A | 306 | 37.722 | 8.751  | 34.650 | 1.000 | 60.08  |
| ATOM | 2350 | N   | ALA | A | 307 | 36.073 | 7.760  | 35.834 | 1.000 | 70.13  |
| ATOM | 2351 | CA  | ALA | A | 307 | 36.735 | 6.475  | 36.013 | 1.000 | 72.89  |
| ATOM | 2352 | CB  | ALA | A | 307 | 35.766 | 5.449  | 36.576 | 1.000 | 79.56  |
| ATOM | 2353 | C   | ALA | A | 307 | 37.324 | 5.984  | 34.694 | 1.000 | 75.87  |
| ATOM | 2354 | O   | ALA | A | 307 | 38.449 | 5.491  | 34.642 | 1.000 | 86.48  |
| ATOM | 2355 | N   | ARG | A | 308 | 36.535 | 6.146  | 33.635 | 1.000 | 72.53  |
| ATOM | 2356 | CA  | ARG | A | 308 | 36.980 | 5.843  | 32.285 | 1.000 | 71.87  |
| ATOM | 2357 | CB  | ARG | A | 308 | 35.954 | 6.318  | 31.260 | 1.000 | 72.41  |
| ATOM | 2358 | CG  | ARG | A | 308 | 35.892 | 5.489  | 29.991 | 1.000 | 75.31  |
| ATOM | 2359 | CD  | ARG | A | 308 | 34.468 | 5.480  | 29.453 | 1.000 | 81.76  |
| ATOM | 2360 | NE  | ARG | A | 308 | 34.286 | 4.508  | 28.381 | 1.000 | 82.26  |
| ATOM | 2361 | CZ  | ARG | A | 308 | 33.963 | 4.835  | 27.136 | 1.000 | 81.15  |
| ATOM | 2362 | NH1 | ARG | A | 308 | 33.794 | 6.106  | 26.802 | 1.000 | 66.44  |
| ATOM | 2363 | NH2 | ARG | A | 308 | 33.818 | 3.879  | 26.222 | 1.000 | 98.94  |
| ATOM | 2364 | C   | ARG | A | 308 | 38.316 | 6.522  | 31.997 | 1.000 | 79.31  |
| ATOM | 2365 | O   | ARG | A | 308 | 39.323 | 6.227  | 32.636 | 1.000 | 93.34  |
| ATOM | 2366 | N   | LYS | A | 309 | 38.277 | 7.433  | 31.039 | 1.000 | 83.39  |
| ATOM | 2367 | CA  | LYS | A | 309 | 39.434 | 8.214  | 30.626 | 1.000 | 85.77  |
| ATOM | 2368 | CB  | LYS | A | 309 | 39.029 | 9.196  | 29.532 | 1.000 | 85.52  |
| ATOM | 2369 | CG  | LYS | A | 309 | 37.652 | 8.903  | 28.934 | 1.000 | 85.90  |
| ATOM | 2370 | CD  | LYS | A | 309 | 36.903 | 10.189 | 28.611 | 1.000 | 87.13  |
| ATOM | 2371 | CE  | LYS | A | 309 | 37.828 | 11.241 | 28.041 | 1.000 | 90.18  |
| ATOM | 2372 | NZ  | LYS | A | 309 | 37.294 | 11.834 | 26.782 | 1.000 | 95.87  |
| ATOM | 2373 | C   | LYS | A | 309 | 40.045 | 8.948  | 31.819 | 1.000 | 88.05  |
| ATOM | 2374 | O   | LYS | A | 309 | 39.829 | 10.143 | 32.007 | 1.000 | 83.82  |
| ATOM | 2375 | N   | LEU | A | 310 | 40.812 | 8.199  | 32.602 | 1.000 | 91.25  |
| ATOM | 2376 | CA  | LEU | A | 310 | 41.488 | 8.642  | 33.803 | 1.000 | 89.65  |
| ATOM | 2377 | CB  | LEU | A | 310 | 40.575 | 8.511  | 35.031 | 1.000 | 89.61  |
| ATOM | 2378 | CG  | LEU | A | 310 | 41.209 | 8.874  | 36.375 | 1.000 | 91.78  |
| ATOM | 2379 | CD1 | LEU | A | 310 | 41.928 | 10.213 | 36.280 | 1.000 | 97.42  |
| ATOM | 2380 | CD2 | LEU | A | 310 | 40.167 | 8.896  | 37.476 | 1.000 | 97.23  |
| ATOM | 2381 | C   | LEU | A | 310 | 42.772 | 7.848  | 34.034 | 1.000 | 88.08  |
| ATOM | 2382 | O   | LEU | A | 310 | 42.708 | 6.719  | 34.516 | 1.000 | 91.11  |
| ATOM | 2383 | N   | LYS | B | 19  | 45.803 | 11.373 | 51.943 | 1.000 | 103.56 |
| ATOM | 2384 | CA  | LYS | B | 19  | 45.533 | 10.011 | 51.483 | 1.000 | 77.94  |
| ATOM | 2385 | CB  | LYS | B | 19  | 46.473 | 9.008  | 52.147 | 1.000 | 82.60  |
| ATOM | 2386 | CG  | LYS | B | 19  | 46.882 | 7.835  | 51.255 | 1.000 | 87.87  |
| ATOM | 2387 | CD  | LYS | B | 19  | 48.286 | 7.354  | 51.584 | 1.000 | 91.26  |
| ATOM | 2388 | CE  | LYS | B | 19  | 49.120 | 7.117  | 50.329 | 1.000 | 90.51  |
| ATOM | 2389 | NZ  | LYS | B | 19  | 50.584 | 7.099  | 50.628 | 1.000 | 76.07  |
| ATOM | 2390 | C   | LYS | B | 19  | 44.082 | 9.614  | 51.751 | 1.000 | 64.77  |
| ATOM | 2391 | O   | LYS | B | 19  | 43.153 | 10.321 | 51.368 | 1.000 | 54.90  |

**FIGURE 52**



|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2392 | N   | THR | B | 20 | 43.927 | 8.473  | 52.402 | 1.000 | 58.60 |
| ATOM | 2393 | CA  | THR | B | 20 | 42.644 | 7.870  | 52.709 | 1.000 | 50.23 |
| ATOM | 2394 | CB  | THR | B | 20 | 42.853 | 6.643  | 53.618 | 1.000 | 48.19 |
| ATOM | 2395 | OG1 | THR | B | 20 | 41.626 | 6.256  | 54.241 | 1.000 | 67.26 |
| ATOM | 2396 | CG2 | THR | B | 20 | 43.824 | 6.994  | 54.737 | 1.000 | 41.73 |
| ATOM | 2397 | C   | THR | B | 20 | 41.695 | 8.862  | 53.376 | 1.000 | 54.14 |
| ATOM | 2398 | O   | THR | B | 20 | 42.126 | 9.839  | 53.992 | 1.000 | 48.50 |
| ATOM | 2399 | N   | SER | B | 21 | 40.407 | 8.579  | 53.235 | 1.000 | 57.41 |
| ATOM | 2400 | CA  | SER | B | 21 | 39.308 | 9.335  | 53.812 | 1.000 | 54.62 |
| ATOM | 2401 | CB  | SER | B | 21 | 39.008 | 10.562 | 52.951 | 1.000 | 57.73 |
| ATOM | 2402 | OG  | SER | B | 21 | 38.000 | 10.316 | 51.989 | 1.000 | 61.68 |
| ATOM | 2403 | C   | SER | B | 21 | 38.071 | 8.452  | 53.980 | 1.000 | 51.70 |
| ATOM | 2404 | O   | SER | B | 21 | 38.044 | 7.306  | 53.523 | 1.000 | 45.33 |
| ATOM | 2405 | N   | CYS | B | 22 | 37.038 | 8.961  | 54.640 | 1.000 | 48.54 |
| ATOM | 2406 | CA  | CYS | B | 22 | 35.824 | 8.195  | 54.908 | 1.000 | 41.60 |
| ATOM | 2407 | CB  | CYS | B | 22 | 35.884 | 7.524  | 56.281 | 1.000 | 46.98 |
| ATOM | 2408 | SG  | CYS | B | 22 | 36.813 | 5.974  | 56.365 | 1.000 | 93.30 |
| ATOM | 2409 | C   | CYS | B | 22 | 34.590 | 9.082  | 54.851 | 1.000 | 38.62 |
| ATOM | 2410 | O   | CYS | B | 22 | 34.027 | 9.443  | 55.887 | 1.000 | 49.86 |
| ATOM | 2411 | N   | PRO | B | 23 | 34.143 | 9.447  | 53.659 | 1.000 | 47.14 |
| ATOM | 2412 | CA  | PRO | B | 23 | 32.954 | 10.304 | 53.566 | 1.000 | 56.35 |
| ATOM | 2413 | CB  | PRO | B | 23 | 32.868 | 10.652 | 52.085 | 1.000 | 55.14 |
| ATOM | 2414 | CG  | PRO | B | 23 | 34.157 | 10.216 | 51.473 | 1.000 | 48.26 |
| ATOM | 2415 | CD  | PRO | B | 23 | 34.680 | 9.104  | 52.334 | 1.000 | 45.23 |
| ATOM | 2416 | C   | PRO | B | 23 | 31.720 | 9.529  | 54.021 | 1.000 | 59.08 |
| ATOM | 2417 | O   | PRO | B | 23 | 31.566 | 8.358  | 53.677 | 1.000 | 63.26 |
| ATOM | 2418 | N   | ILE | B | 24 | 30.856 | 10.175 | 54.800 | 1.000 | 57.72 |
| ATOM | 2419 | CA  | ILE | B | 24 | 29.645 | 9.515  | 55.274 | 1.000 | 57.66 |
| ATOM | 2420 | CB  | ILE | B | 24 | 29.730 | 9.129  | 56.761 | 1.000 | 61.40 |
| ATOM | 2421 | CG1 | ILE | B | 24 | 30.656 | 7.951  | 57.048 | 1.000 | 63.99 |
| ATOM | 2422 | CD1 | ILE | B | 24 | 31.645 | 8.269  | 58.170 | 1.000 | 72.75 |
| ATOM | 2423 | CG2 | ILE | B | 24 | 28.346 | 8.849  | 57.336 | 1.000 | 55.60 |
| ATOM | 2424 | C   | ILE | B | 24 | 28.423 | 10.404 | 55.073 | 1.000 | 56.32 |
| ATOM | 2425 | O   | ILE | B | 24 | 28.463 | 11.607 | 55.319 | 1.000 | 56.42 |
| ATOM | 2426 | N   | LYS | B | 25 | 27.336 | 9.790  | 54.618 | 1.000 | 60.08 |
| ATOM | 2427 | CA  | LYS | B | 25 | 26.083 | 10.506 | 54.431 | 1.000 | 69.15 |
| ATOM | 2428 | CB  | LYS | B | 25 | 24.998 | 9.583  | 53.874 | 1.000 | 82.75 |
| ATOM | 2429 | CG  | LYS | B | 25 | 25.033 | 9.350  | 52.369 | 1.000 | 85.99 |
| ATOM | 2430 | CD  | LYS | B | 25 | 24.777 | 7.874  | 52.048 | 1.000 | 85.92 |
| ATOM | 2431 | CE  | LYS | B | 25 | 26.083 | 7.172  | 51.689 | 1.000 | 85.44 |
| ATOM | 2432 | NZ  | LYS | B | 25 | 26.510 | 7.499  | 50.285 | 1.000 | 80.54 |
| ATOM | 2433 | C   | LYS | B | 25 | 25.604 | 11.112 | 55.747 | 1.000 | 63.20 |
| ATOM | 2434 | O   | LYS | B | 25 | 25.591 | 10.438 | 56.783 | 1.000 | 50.64 |
| ATOM | 2435 | N   | ILE | B | 26 | 25.195 | 12.378 | 55.680 | 1.000 | 54.67 |
| ATOM | 2436 | CA  | ILE | B | 26 | 24.670 | 13.059 | 56.860 | 1.000 | 55.87 |
| ATOM | 2437 | CB  | ILE | B | 26 | 24.575 | 14.581 | 56.678 | 1.000 | 58.65 |
| ATOM | 2438 | CG1 | ILE | B | 26 | 23.569 | 15.042 | 55.620 | 1.000 | 60.19 |
| ATOM | 2439 | CD1 | ILE | B | 26 | 23.370 | 16.547 | 55.610 | 1.000 | 57.06 |
| ATOM | 2440 | CG2 | ILE | B | 26 | 25.953 | 15.157 | 56.389 | 1.000 | 63.31 |
| ATOM | 2441 | C   | ILE | B | 26 | 23.291 | 12.498 | 57.214 | 1.000 | 58.06 |
| ATOM | 2442 | O   | ILE | B | 26 | 22.810 | 12.724 | 58.319 | 1.000 | 56.98 |
| ATOM | 2443 | N   | ASN | B | 27 | 22.730 | 11.784 | 56.260 | 1.000 | 61.16 |

**FIGURE 53**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |        |
|------|------|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 2444 | CA  | ASN | B | 27 | 21.489 | 11.049 | 56.299 | 1.000 | 59.75  |
| ATOM | 2445 | CB  | ASN | B | 27 | 21.008 | 10.743 | 54.876 | 1.000 | 63.07  |
| ATOM | 2446 | CG  | ASN | B | 27 | 20.656 | 12.000 | 54.106 | 1.000 | 65.31  |
| ATOM | 2447 | OD1 | ASN | B | 27 | 20.305 | 11.913 | 52.930 | 1.000 | 50.97  |
| ATOM | 2448 | ND2 | ASN | B | 27 | 20.748 | 13.143 | 54.774 | 1.000 | 75.32  |
| ATOM | 2449 | C   | ASN | B | 27 | 21.632 | 9.724  | 57.040 | 1.000 | 57.11  |
| ATOM | 2450 | O   | ASN | B | 27 | 20.646 | 9.183  | 57.534 | 1.000 | 57.56  |
| ATOM | 2451 | N   | GLN | B | 28 | 22.856 | 9.217  | 57.094 | 1.000 | 57.63  |
| ATOM | 2452 | CA  | GLN | B | 28 | 23.130 | 7.930  | 57.717 | 1.000 | 56.91  |
| ATOM | 2453 | CB  | GLN | B | 28 | 23.761 | 6.988  | 56.678 | 1.000 | 64.21  |
| ATOM | 2454 | CG  | GLN | B | 28 | 24.000 | 5.578  | 57.192 | 1.000 | 66.30  |
| ATOM | 2455 | CD  | GLN | B | 28 | 22.771 | 4.698  | 57.075 | 1.000 | 70.95  |
| ATOM | 2456 | OE1 | GLN | B | 28 | 22.005 | 4.829  | 56.119 | 1.000 | 74.56  |
| ATOM | 2457 | NE2 | GLN | B | 28 | 22.580 | 3.801  | 58.039 | 1.000 | 63.57  |
| ATOM | 2458 | C   | GLN | B | 28 | 24.053 | 8.043  | 58.917 | 1.000 | 44.81  |
| ATOM | 2459 | O   | GLN | B | 28 | 24.358 | 7.034  | 59.556 | 1.000 | 48.39  |
| ATOM | 2460 | N   | PHE | B | 29 | 24.526 | 9.244  | 59.241 | 1.000 | 46.88  |
| ATOM | 2461 | CA  | PHE | B | 29 | 25.544 | 9.393  | 60.273 | 1.000 | 36.76  |
| ATOM | 2462 | CB  | PHE | B | 29 | 25.849 | 10.882 | 60.532 | 1.000 | 43.65  |
| ATOM | 2463 | CG  | PHE | B | 29 | 27.092 | 11.033 | 61.384 | 1.000 | 41.38  |
| ATOM | 2464 | CD1 | PHE | B | 29 | 28.348 | 10.939 | 60.813 | 1.000 | 39.51  |
| ATOM | 2465 | CE1 | PHE | B | 29 | 29.493 | 11.073 | 61.579 | 1.000 | 39.09  |
| ATOM | 2466 | CZ  | PHE | B | 29 | 29.383 | 11.303 | 62.933 | 1.000 | 38.33  |
| ATOM | 2467 | CE2 | PHE | B | 29 | 28.131 | 11.392 | 63.518 | 1.000 | 42.37  |
| ATOM | 2468 | CD2 | PHE | B | 29 | 26.995 | 11.257 | 62.747 | 1.000 | 38.83  |
| ATOM | 2469 | C   | PHE | B | 29 | 25.186 | 8.747  | 61.601 | 1.000 | 37.74  |
| ATOM | 2470 | O   | PHE | B | 29 | 26.032 | 8.087  | 62.213 | 1.000 | 43.72  |
| ATOM | 2471 | N   | GLU | B | 30 | 23.960 | 8.933  | 62.080 | 1.000 | 45.93  |
| ATOM | 2472 | CA  | GLU | B | 30 | 23.554 | 8.292  | 63.331 | 1.000 | 49.96  |
| ATOM | 2473 | CB  | GLU | B | 30 | 22.082 | 8.589  | 63.614 | 1.000 | 61.18  |
| ATOM | 2474 | CG  | GLU | B | 30 | 21.655 | 8.277  | 65.041 | 1.000 | 72.30  |
| ATOM | 2475 | CD  | GLU | B | 30 | 22.517 | 8.965  | 66.069 | 1.000 | 84.23  |
| ATOM | 2476 | OE1 | GLU | B | 30 | 23.748 | 8.742  | 66.082 | 1.000 | 104.41 |
| ATOM | 2477 | OE2 | GLU | B | 30 | 21.962 | 9.740  | 66.892 | 1.000 | 90.78  |
| ATOM | 2478 | C   | GLU | B | 30 | 23.801 | 6.785  | 63.292 | 1.000 | 53.76  |
| ATOM | 2479 | O   | GLU | B | 30 | 24.396 | 6.207  | 64.208 | 1.000 | 40.13  |
| ATOM | 2480 | N   | GLY | B | 31 | 23.348 | 6.160  | 62.207 | 1.000 | 50.11  |
| ATOM | 2481 | CA  | GLY | B | 31 | 23.552 | 4.743  | 61.979 | 1.000 | 39.81  |
| ATOM | 2482 | C   | GLY | B | 31 | 25.024 | 4.352  | 61.975 | 1.000 | 42.21  |
| ATOM | 2483 | O   | GLY | B | 31 | 25.429 | 3.569  | 62.841 | 1.000 | 48.72  |
| ATOM | 2484 | N   | HIS | B | 32 | 25.786 | 4.891  | 61.027 | 1.000 | 44.34  |
| ATOM | 2485 | CA  | HIS | B | 32 | 27.227 | 4.682  | 60.898 | 1.000 | 44.47  |
| ATOM | 2486 | CB  | HIS | B | 32 | 27.848 | 5.622  | 59.865 | 1.000 | 46.08  |
| ATOM | 2487 | CG  | HIS | B | 32 | 29.339 | 5.758  | 59.929 | 1.000 | 57.10  |
| ATOM | 2488 | ND1 | HIS | B | 32 | 30.199 | 4.924  | 59.241 | 1.000 | 54.47  |
| ATOM | 2489 | CE1 | HIS | B | 32 | 31.451 | 5.291  | 59.477 | 1.000 | 52.58  |
| ATOM | 2490 | NE2 | HIS | B | 32 | 31.440 | 6.328  | 60.296 | 1.000 | 49.52  |
| ATOM | 2491 | CD2 | HIS | B | 32 | 30.140 | 6.650  | 60.573 | 1.000 | 56.38  |
| ATOM | 2492 | C   | HIS | B | 32 | 27.916 | 4.872  | 62.244 | 1.000 | 43.34  |
| ATOM | 2493 | O   | HIS | B | 32 | 28.702 | 4.051  | 62.710 | 1.000 | 44.29  |
| ATOM | 2494 | N   | PHE | B | 33 | 27.608 | 6.001  | 62.884 | 1.000 | 42.64  |
| ATOM | 2495 | CA  | PHE | B | 33 | 28.186 | 6.230  | 64.209 | 1.000 | 46.60  |

**FIGURE 54**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2496 | CB  | PHE | B | 33 | 27.794 | 7.621  | 64.705 | 1.000 | 45.66 |
| ATOM | 2497 | CG  | PHE | B | 33 | 28.411 | 8.010  | 66.024 | 1.000 | 41.60 |
| ATOM | 2498 | CD1 | PHE | B | 33 | 29.639 | 7.503  | 66.418 | 1.000 | 28.55 |
| ATOM | 2499 | CE1 | PHE | B | 33 | 30.180 | 7.856  | 67.635 | 1.000 | 34.17 |
| ATOM | 2500 | CZ  | PHE | B | 33 | 29.502 | 8.729  | 68.464 | 1.000 | 39.16 |
| ATOM | 2501 | CE2 | PHE | B | 33 | 28.282 | 9.249  | 68.088 | 1.000 | 40.43 |
| ATOM | 2502 | CD2 | PHE | B | 33 | 27.743 | 8.885  | 66.871 | 1.000 | 46.28 |
| ATOM | 2503 | C   | PHE | B | 33 | 27.742 | 5.122  | 65.157 | 1.000 | 49.56 |
| ATOM | 2504 | O   | PHE | B | 33 | 28.543 | 4.568  | 65.918 | 1.000 | 39.50 |
| ATOM | 2505 | N   | MET | B | 34 | 26.451 | 4.782  | 65.110 | 1.000 | 53.61 |
| ATOM | 2506 | CA  | MET | B | 34 | 25.979 | 3.673  | 65.946 | 1.000 | 51.72 |
| ATOM | 2507 | CB  | MET | B | 34 | 24.456 | 3.545  | 65.882 | 1.000 | 51.72 |
| ATOM | 2508 | CG  | MET | B | 34 | 23.750 | 4.565  | 66.777 | 1.000 | 52.01 |
| ATOM | 2509 | SD  | MET | B | 34 | 22.105 | 4.050  | 67.305 | 1.000 | 72.48 |
| ATOM | 2510 | CE  | MET | B | 34 | 21.721 | 2.817  | 66.063 | 1.000 | 45.79 |
| ATOM | 2511 | C   | MET | B | 34 | 26.671 | 2.377  | 65.554 | 1.000 | 52.65 |
| ATOM | 2512 | O   | MET | B | 34 | 27.064 | 1.601  | 66.433 | 1.000 | 63.08 |
| ATOM | 2513 | N   | LYS | B | 35 | 26.862 | 2.114  | 64.258 | 1.000 | 52.00 |
| ATOM | 2514 | CA  | LYS | B | 35 | 27.584 | 0.889  | 63.905 | 1.000 | 54.31 |
| ATOM | 2515 | CB  | LYS | B | 35 | 27.570 | 0.627  | 62.402 | 1.000 | 59.44 |
| ATOM | 2516 | CG  | LYS | B | 35 | 26.633 | 1.515  | 61.614 | 1.000 | 66.12 |
| ATOM | 2517 | CD  | LYS | B | 35 | 26.520 | 1.074  | 60.166 | 1.000 | 69.40 |
| ATOM | 2518 | CE  | LYS | B | 35 | 25.639 | 2.012  | 59.351 | 1.000 | 62.69 |
| ATOM | 2519 | NZ  | LYS | B | 35 | 26.251 | 2.293  | 58.019 | 1.000 | 48.67 |
| ATOM | 2520 | C   | LYS | B | 35 | 29.028 | 0.951  | 64.404 | 1.000 | 56.64 |
| ATOM | 2521 | O   | LYS | B | 35 | 29.607 | -0.094 | 64.699 | 1.000 | 47.38 |
| ATOM | 2522 | N   | LEU | B | 36 | 29.564 | 2.163  | 64.485 | 1.000 | 61.24 |
| ATOM | 2523 | CA  | LEU | B | 36 | 30.933 | 2.424  | 64.902 | 1.000 | 59.97 |
| ATOM | 2524 | CB  | LEU | B | 36 | 31.323 | 3.874  | 64.594 | 1.000 | 64.56 |
| ATOM | 2525 | CG  | LEU | B | 36 | 32.434 | 4.056  | 63.557 | 1.000 | 65.01 |
| ATOM | 2526 | CD1 | LEU | B | 36 | 32.294 | 3.032  | 62.440 | 1.000 | 65.86 |
| ATOM | 2527 | CD2 | LEU | B | 36 | 32.421 | 5.477  | 63.006 | 1.000 | 46.61 |
| ATOM | 2528 | C   | LEU | B | 36 | 31.155 | 2.157  | 66.385 | 1.000 | 58.41 |
| ATOM | 2529 | O   | LEU | B | 36 | 32.238 | 1.731  | 66.790 | 1.000 | 42.70 |
| ATOM | 2530 | N   | GLN | B | 37 | 30.143 | 2.412  | 67.207 | 1.000 | 64.59 |
| ATOM | 2531 | CA  | GLN | B | 37 | 30.253 | 2.093  | 68.627 | 1.000 | 66.89 |
| ATOM | 2532 | CB  | GLN | B | 37 | 29.379 | 3.009  | 69.479 | 1.000 | 65.39 |
| ATOM | 2533 | CG  | GLN | B | 37 | 29.268 | 4.435  | 68.963 | 1.000 | 71.01 |
| ATOM | 2534 | CD  | GLN | B | 37 | 29.402 | 5.459  | 70.075 | 1.000 | 69.30 |
| ATOM | 2535 | OE1 | GLN | B | 37 | 28.554 | 6.349  | 70.194 | 1.000 | 65.62 |
| ATOM | 2536 | NE2 | GLN | B | 37 | 30.448 | 5.336  | 70.883 | 1.000 | 67.63 |
| ATOM | 2537 | C   | GLN | B | 37 | 29.858 | 0.639  | 68.887 | 1.000 | 64.12 |
| ATOM | 2538 | O   | GLN | B | 37 | 30.133 | 0.109  | 69.965 | 1.000 | 61.41 |
| ATOM | 2539 | N   | ALA | B | 38 | 29.211 | 0.013  | 67.912 | 1.000 | 61.52 |
| ATOM | 2540 | CA  | ALA | B | 38 | 28.752 | -1.364 | 68.068 | 1.000 | 61.79 |
| ATOM | 2541 | CB  | ALA | B | 38 | 27.973 | -1.811 | 66.843 | 1.000 | 61.12 |
| ATOM | 2542 | C   | ALA | B | 38 | 29.924 | -2.304 | 68.328 | 1.000 | 71.64 |
| ATOM | 2543 | O   | ALA | B | 38 | 31.070 | -1.992 | 68.000 | 1.000 | 88.33 |
| ATOM | 2544 | N   | ASP | B | 39 | 29.627 | -3.453 | 68.927 | 1.000 | 75.20 |
| ATOM | 2545 | CA  | ASP | B | 39 | 30.678 | -4.382 | 69.332 | 1.000 | 79.52 |
| ATOM | 2546 | CB  | ASP | B | 39 | 31.399 | -4.960 | 68.119 | 1.000 | 83.70 |
| ATOM | 2547 | CG  | ASP | B | 39 | 31.928 | -6.362 | 68.329 | 1.000 | 85.54 |

**FIGURE 55**

|      |      |     |     |   |    |        |        |        |       |        |
|------|------|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 2548 | OD1 | ASP | B | 39 | 33.151 | -6.572 | 68.165 | 1.000 | 77.07  |
| ATOM | 2549 | OD2 | ASP | B | 39 | 31.125 | -7.261 | 68.656 | 1.000 | 94.95  |
| ATOM | 2550 | C   | ASP | B | 39 | 31.654 | -3.661 | 70.262 | 1.000 | 80.16  |
| ATOM | 2551 | O   | ASP | B | 39 | 32.866 | -3.844 | 70.171 | 1.000 | 82.76  |
| ATOM | 2552 | N   | SER | B | 40 | 31.091 | -2.847 | 71.149 | 1.000 | 80.57  |
| ATOM | 2553 | CA  | SER | B | 40 | 31.845 | -2.060 | 72.117 | 1.000 | 88.50  |
| ATOM | 2554 | CB  | SER | B | 40 | 32.474 | -2.960 | 73.184 | 1.000 | 94.68  |
| ATOM | 2555 | OG  | SER | B | 40 | 32.154 | -2.503 | 74.493 | 1.000 | 104.32 |
| ATOM | 2556 | C   | SER | B | 40 | 32.923 | -1.227 | 71.430 | 1.000 | 88.12  |
| ATOM | 2557 | O   | SER | B | 40 | 34.120 | -1.492 | 71.558 | 1.000 | 101.21 |
| ATOM | 2558 | N   | ASN | B | 41 | 32.493 | -0.212 | 70.685 | 1.000 | 79.40  |
| ATOM | 2559 | CA  | ASN | B | 41 | 33.401 | 0.680  | 69.978 | 1.000 | 77.46  |
| ATOM | 2560 | CB  | ASN | B | 41 | 34.193 | 1.538  | 70.973 | 1.000 | 73.13  |
| ATOM | 2561 | CG  | ASN | B | 41 | 33.910 | 3.013  | 70.761 | 1.000 | 66.31  |
| ATOM | 2562 | OD1 | ASN | B | 41 | 32.852 | 3.359  | 70.237 | 1.000 | 66.52  |
| ATOM | 2563 | ND2 | ASN | B | 41 | 34.853 | 3.853  | 71.161 | 1.000 | 67.42  |
| ATOM | 2564 | C   | ASN | B | 41 | 34.370 | -0.080 | 69.091 | 1.000 | 78.31  |
| ATOM | 2565 | O   | ASN | B | 41 | 35.499 | 0.345  | 68.837 | 1.000 | 79.80  |
| ATOM | 2566 | N   | TYR | B | 42 | 33.919 | -1.239 | 68.605 | 1.000 | 74.28  |
| ATOM | 2567 | CA  | TYR | B | 42 | 34.837 | -2.034 | 67.800 | 1.000 | 72.73  |
| ATOM | 2568 | CB  | TYR | B | 42 | 34.211 | -3.377 | 67.423 | 1.000 | 73.56  |
| ATOM | 2569 | CG  | TYR | B | 42 | 35.147 | -4.228 | 66.588 | 1.000 | 73.21  |
| ATOM | 2570 | CD1 | TYR | B | 42 | 36.311 | -4.738 | 67.144 | 1.000 | 77.06  |
| ATOM | 2571 | CE1 | TYR | B | 42 | 37.173 | -5.514 | 66.388 | 1.000 | 78.96  |
| ATOM | 2572 | CZ  | TYR | B | 42 | 36.872 | -5.773 | 65.067 | 1.000 | 78.31  |
| ATOM | 2573 | OH  | TYR | B | 42 | 37.729 | -6.541 | 64.312 | 1.000 | 91.83  |
| ATOM | 2574 | CE2 | TYR | B | 42 | 35.724 | -5.272 | 64.492 | 1.000 | 73.89  |
| ATOM | 2575 | CD2 | TYR | B | 42 | 34.868 | -4.501 | 65.256 | 1.000 | 72.17  |
| ATOM | 2576 | C   | TYR | B | 42 | 35.257 | -1.247 | 66.561 | 1.000 | 64.17  |
| ATOM | 2577 | O   | TYR | B | 42 | 36.414 | -0.843 | 66.456 | 1.000 | 62.76  |
| ATOM | 2578 | N   | LEU | B | 43 | 34.312 | -1.041 | 65.653 | 1.000 | 59.26  |
| ATOM | 2579 | CA  | LEU | B | 43 | 34.589 | -0.428 | 64.362 | 1.000 | 59.76  |
| ATOM | 2580 | CB  | LEU | B | 43 | 33.310 | -0.304 | 63.528 | 1.000 | 63.25  |
| ATOM | 2581 | CG  | LEU | B | 43 | 32.890 | -1.570 | 62.775 | 1.000 | 63.42  |
| ATOM | 2582 | CD1 | LEU | B | 43 | 31.436 | -1.480 | 62.336 | 1.000 | 46.05  |
| ATOM | 2583 | CD2 | LEU | B | 43 | 33.807 | -1.812 | 61.585 | 1.000 | 76.10  |
| ATOM | 2584 | C   | LEU | B | 43 | 35.252 | 0.932  | 64.522 | 1.000 | 54.62  |
| ATOM | 2585 | O   | LEU | B | 43 | 36.208 | 1.237  | 63.810 | 1.000 | 53.46  |
| ATOM | 2586 | N   | LEU | B | 44 | 34.760 | 1.742  | 65.454 | 1.000 | 56.15  |
| ATOM | 2587 | CA  | LEU | B | 44 | 35.409 | 3.030  | 65.682 | 1.000 | 52.24  |
| ATOM | 2588 | CB  | LEU | B | 44 | 34.729 | 3.785  | 66.826 | 1.000 | 48.36  |
| ATOM | 2589 | CG  | LEU | B | 44 | 35.293 | 5.195  | 67.068 | 1.000 | 49.68  |
| ATOM | 2590 | CD1 | LEU | B | 44 | 35.267 | 6.017  | 65.787 | 1.000 | 41.86  |
| ATOM | 2591 | CD2 | LEU | B | 44 | 34.522 | 5.886  | 68.170 | 1.000 | 38.98  |
| ATOM | 2592 | C   | LEU | B | 44 | 36.898 | 2.865  | 65.975 | 1.000 | 48.68  |
| ATOM | 2593 | O   | LEU | B | 44 | 37.732 | 3.549  | 65.378 | 1.000 | 45.89  |
| ATOM | 2594 | N   | SER | B | 45 | 37.242 | 1.962  | 66.882 | 1.000 | 49.23  |
| ATOM | 2595 | CA  | SER | B | 45 | 38.619 | 1.713  | 67.282 | 1.000 | 39.06  |
| ATOM | 2596 | CB  | SER | B | 45 | 38.690 | 0.436  | 68.127 | 1.000 | 39.80  |
| ATOM | 2597 | OG  | SER | B | 45 | 39.247 | 0.727  | 69.398 | 1.000 | 49.93  |
| ATOM | 2598 | C   | SER | B | 45 | 39.558 | 1.552  | 66.098 | 1.000 | 45.56  |
| ATOM | 2599 | O   | SER | B | 45 | 40.668 | 2.082  | 66.083 | 1.000 | 52.78  |

FIGURE 56

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |        |
|------|------|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 2600 | N   | LYS | B | 46 | 39.087 | 0.795  | 65.113 | 1.000 | 51.54  |
| ATOM | 2601 | CA  | LYS | B | 46 | 39.891 | 0.470  | 63.941 | 1.000 | 63.73  |
| ATOM | 2602 | CB  | LYS | B | 46 | 39.189 | -0.575 | 63.073 | 1.000 | 74.89  |
| ATOM | 2603 | CG  | LYS | B | 46 | 39.589 | -2.009 | 63.395 | 1.000 | 86.82  |
| ATOM | 2604 | CD  | LYS | B | 46 | 39.920 | -2.808 | 62.129 | 1.000 | 98.47  |
| ATOM | 2605 | CE  | LYS | B | 46 | 40.285 | -4.250 | 62.467 | 1.000 | 105.16 |
| ATOM | 2606 | NZ  | LYS | B | 46 | 39.701 | -5.221 | 61.446 | 1.000 | 118.97 |
| ATOM | 2607 | C   | LYS | B | 46 | 40.196 | 1.720  | 63.115 | 1.000 | 64.75  |
| ATOM | 2608 | O   | LYS | B | 46 | 41.369 | 2.039  | 62.917 | 1.000 | 80.74  |
| ATOM | 2609 | N   | GLU | B | 47 | 39.144 | 2.386  | 62.661 | 1.000 | 60.32  |
| ATOM | 2610 | CA  | GLU | B | 47 | 39.214 | 3.608  | 61.876 | 1.000 | 57.31  |
| ATOM | 2611 | CB  | GLU | B | 47 | 37.861 | 4.317  | 61.829 | 1.000 | 59.96  |
| ATOM | 2612 | CG  | GLU | B | 47 | 37.108 | 4.262  | 60.513 | 1.000 | 64.86  |
| ATOM | 2613 | CD  | GLU | B | 47 | 36.069 | 5.368  | 60.394 | 1.000 | 62.05  |
| ATOM | 2614 | OE1 | GLU | B | 47 | 35.086 | 5.213  | 59.637 | 1.000 | 43.75  |
| ATOM | 2615 | OE2 | GLU | B | 47 | 36.243 | 6.408  | 61.066 | 1.000 | 56.16  |
| ATOM | 2616 | C   | GLU | B | 47 | 40.261 | 4.566  | 62.445 | 1.000 | 52.08  |
| ATOM | 2617 | O   | GLU | B | 47 | 40.973 | 5.207  | 61.673 | 1.000 | 46.49  |
| ATOM | 2618 | N   | TYR | B | 48 | 40.331 | 4.643  | 63.772 | 1.000 | 51.35  |
| ATOM | 2619 | CA  | TYR | B | 48 | 41.241 | 5.559  | 64.447 | 1.000 | 47.41  |
| ATOM | 2620 | CB  | TYR | B | 48 | 40.768 | 5.841  | 65.876 | 1.000 | 43.35  |
| ATOM | 2621 | CG  | TYR | B | 48 | 41.664 | 6.800  | 66.628 | 1.000 | 43.06  |
| ATOM | 2622 | CD1 | TYR | B | 48 | 41.634 | 8.162  | 66.350 | 1.000 | 43.39  |
| ATOM | 2623 | CE1 | TYR | B | 48 | 42.446 | 9.049  | 67.026 | 1.000 | 33.55  |
| ATOM | 2624 | CZ  | TYR | B | 48 | 43.301 | 8.577  | 67.997 | 1.000 | 33.43  |
| ATOM | 2625 | OH  | TYR | B | 48 | 44.109 | 9.457  | 68.675 | 1.000 | 39.28  |
| ATOM | 2626 | CE2 | TYR | B | 48 | 43.357 | 7.232  | 68.299 | 1.000 | 35.45  |
| ATOM | 2627 | CD2 | TYR | B | 48 | 42.538 | 6.354  | 67.609 | 1.000 | 39.88  |
| ATOM | 2628 | C   | TYR | B | 48 | 42.666 | 5.026  | 64.486 | 1.000 | 44.84  |
| ATOM | 2629 | O   | TYR | B | 48 | 43.636 | 5.779  | 64.556 | 1.000 | 38.45  |
| ATOM | 2630 | N   | GLU | B | 49 | 42.798 | 3.704  | 64.448 | 1.000 | 45.22  |
| ATOM | 2631 | CA  | GLU | B | 49 | 44.131 | 3.103  | 64.459 | 1.000 | 46.18  |
| ATOM | 2632 | CB  | GLU | B | 49 | 44.027 | 1.636  | 64.889 | 1.000 | 60.64  |
| ATOM | 2633 | CG  | GLU | B | 49 | 43.562 | 1.476  | 66.331 | 1.000 | 71.11  |
| ATOM | 2634 | CD  | GLU | B | 49 | 44.096 | 2.572  | 67.234 | 1.000 | 79.66  |
| ATOM | 2635 | OE1 | GLU | B | 49 | 43.360 | 2.978  | 68.161 | 1.000 | 77.35  |
| ATOM | 2636 | OE2 | GLU | B | 49 | 45.242 | 3.035  | 67.029 | 1.000 | 85.01  |
| ATOM | 2637 | C   | GLU | B | 49 | 44.790 | 3.234  | 63.097 | 1.000 | 39.20  |
| ATOM | 2638 | O   | GLU | B | 49 | 46.009 | 3.355  | 62.975 | 1.000 | 46.67  |
| ATOM | 2639 | N   | GLU | B | 50 | 43.971 | 3.230  | 62.044 | 1.000 | 35.49  |
| ATOM | 2640 | CA  | GLU | B | 50 | 44.513 | 3.352  | 60.694 | 1.000 | 43.74  |
| ATOM | 2641 | CB  | GLU | B | 50 | 43.412 | 3.174  | 59.644 | 1.000 | 53.39  |
| ATOM | 2642 | CG  | GLU | B | 50 | 42.601 | 1.900  | 59.756 | 1.000 | 64.71  |
| ATOM | 2643 | CD  | GLU | B | 50 | 41.686 | 1.654  | 58.577 | 1.000 | 72.97  |
| ATOM | 2644 | OE1 | GLU | B | 50 | 41.888 | 0.646  | 57.858 | 1.000 | 85.76  |
| ATOM | 2645 | OE2 | GLU | B | 50 | 40.752 | 2.456  | 58.346 | 1.000 | 70.73  |
| ATOM | 2646 | C   | GLU | B | 50 | 45.205 | 4.698  | 60.485 | 1.000 | 41.38  |
| ATOM | 2647 | O   | GLU | B | 50 | 45.975 | 4.860  | 59.534 | 1.000 | 49.75  |
| ATOM | 2648 | N   | LEU | B | 51 | 44.932 | 5.664  | 61.354 | 1.000 | 32.56  |
| ATOM | 2649 | CA  | LEU | B | 51 | 45.542 | 6.982  | 61.247 | 1.000 | 33.23  |
| ATOM | 2650 | CB  | LEU | B | 51 | 44.611 | 8.073  | 61.767 | 1.000 | 28.37  |
| ATOM | 2651 | CG  | LEU | B | 51 | 43.377 | 8.384  | 60.920 | 1.000 | 34.19  |

**FIGURE 57**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2652 | CD1 | LEU | B | 51 | 42.246 | 8.901  | 61.799 | 1.000 | 37.25 |
| ATOM | 2653 | CD2 | LEU | B | 51 | 43.720 | 9.389  | 59.828 | 1.000 | 48.43 |
| ATOM | 2654 | C   | LEU | B | 51 | 46.840 | 7.056  | 62.042 | 1.000 | 38.45 |
| ATOM | 2655 | O   | LEU | B | 51 | 47.503 | 8.091  | 62.030 | 1.000 | 31.93 |
| ATOM | 2656 | N   | LYS | B | 52 | 47.146 | 5.957  | 62.721 | 1.000 | 40.28 |
| ATOM | 2657 | CA  | LYS | B | 52 | 48.274 | 5.912  | 63.641 | 1.000 | 42.24 |
| ATOM | 2658 | CB  | LYS | B | 52 | 48.513 | 4.470  | 64.104 | 1.000 | 40.97 |
| ATOM | 2659 | CG  | LYS | B | 52 | 49.510 | 4.333  | 65.238 | 1.000 | 42.39 |
| ATOM | 2660 | CD  | LYS | B | 52 | 49.041 | 3.361  | 66.306 | 1.000 | 52.34 |
| ATOM | 2661 | CE  | LYS | B | 52 | 49.390 | 3.867  | 67.700 | 1.000 | 61.04 |
| ATOM | 2662 | NZ  | LYS | B | 52 | 50.844 | 4.180  | 67.830 | 1.000 | 76.71 |
| ATOM | 2663 | C   | LYS | B | 52 | 49.556 | 6.482  | 63.033 | 1.000 | 42.33 |
| ATOM | 2664 | O   | LYS | B | 52 | 50.231 | 7.281  | 63.679 | 1.000 | 51.51 |
| ATOM | 2665 | N   | ASP | B | 53 | 49.860 | 6.073  | 61.826 | 1.000 | 38.71 |
| ATOM | 2666 | CA  | ASP | B | 53 | 51.069 | 6.209  | 61.057 | 1.000 | 45.09 |
| ATOM | 2667 | CB  | ASP | B | 53 | 51.162 | 5.010  | 60.082 | 1.000 | 50.29 |
| ATOM | 2668 | CG  | ASP | B | 53 | 49.852 | 4.773  | 59.352 | 1.000 | 58.20 |
| ATOM | 2669 | OD1 | ASP | B | 53 | 48.816 | 4.532  | 60.008 | 1.000 | 47.71 |
| ATOM | 2670 | OD2 | ASP | B | 53 | 49.828 | 4.823  | 58.101 | 1.000 | 71.83 |
| ATOM | 2671 | C   | ASP | B | 53 | 51.159 | 7.483  | 60.225 | 1.000 | 42.44 |
| ATOM | 2672 | O   | ASP | B | 53 | 52.242 | 7.872  | 59.785 | 1.000 | 38.32 |
| ATOM | 2673 | N   | VAL | B | 54 | 50.014 | 8.111  | 59.996 | 1.000 | 33.25 |
| ATOM | 2674 | CA  | VAL | B | 54 | 49.943 | 9.247  | 59.080 | 1.000 | 30.88 |
| ATOM | 2675 | CB  | VAL | B | 54 | 48.498 | 9.764  | 58.989 | 1.000 | 35.26 |
| ATOM | 2676 | CG1 | VAL | B | 54 | 48.409 | 11.060 | 58.194 | 1.000 | 24.09 |
| ATOM | 2677 | CG2 | VAL | B | 54 | 47.599 | 8.696  | 58.361 | 1.000 | 22.83 |
| ATOM | 2678 | C   | VAL | B | 54 | 50.917 | 10.340 | 59.504 | 1.000 | 32.17 |
| ATOM | 2679 | O   | VAL | B | 54 | 50.929 | 10.809 | 60.638 | 1.000 | 25.64 |
| ATOM | 2680 | N   | GLY | B | 55 | 51.766 | 10.722 | 58.562 | 1.000 | 36.64 |
| ATOM | 2681 | CA  | GLY | B | 55 | 52.749 | 11.767 | 58.654 | 1.000 | 34.77 |
| ATOM | 2682 | C   | GLY | B | 55 | 53.995 | 11.423 | 59.430 | 1.000 | 30.37 |
| ATOM | 2683 | O   | GLY | B | 55 | 54.923 | 12.232 | 59.538 | 1.000 | 25.00 |
| ATOM | 2684 | N   | ARG | B | 56 | 54.036 | 10.221 | 60.001 | 1.000 | 27.19 |
| ATOM | 2685 | CA  | ARG | B | 56 | 55.133 | 9.904  | 60.919 | 1.000 | 34.78 |
| ATOM | 2686 | CB  | ARG | B | 56 | 54.724 | 8.753  | 61.847 | 1.000 | 36.03 |
| ATOM | 2687 | CG  | ARG | B | 56 | 53.643 | 9.120  | 62.851 | 1.000 | 31.22 |
| ATOM | 2688 | CD  | ARG | B | 56 | 54.128 | 10.152 | 63.853 | 1.000 | 34.70 |
| ATOM | 2689 | NE  | ARG | B | 56 | 53.193 | 10.340 | 64.954 | 1.000 | 46.39 |
| ATOM | 2690 | CZ  | ARG | B | 56 | 53.205 | 9.786  | 66.155 | 1.000 | 39.08 |
| ATOM | 2691 | NH1 | ARG | B | 56 | 54.165 | 8.935  | 66.471 | 1.000 | 26.47 |
| ATOM | 2692 | NH2 | ARG | B | 56 | 52.270 | 10.066 | 67.063 | 1.000 | 33.87 |
| ATOM | 2693 | C   | ARG | B | 56 | 56.425 | 9.574  | 60.187 | 1.000 | 37.74 |
| ATOM | 2694 | O   | ARG | B | 56 | 57.415 | 9.186  | 60.808 | 1.000 | 41.64 |
| ATOM | 2695 | N   | ASN | B | 57 | 56.415 | 9.743  | 58.871 | 1.000 | 41.17 |
| ATOM | 2696 | CA  | ASN | B | 57 | 57.583 | 9.563  | 58.028 | 1.000 | 38.70 |
| ATOM | 2697 | CB  | ASN | B | 57 | 57.146 | 9.244  | 56.587 | 1.000 | 42.33 |
| ATOM | 2698 | CG  | ASN | B | 57 | 56.145 | 10.235 | 56.026 | 1.000 | 38.45 |
| ATOM | 2699 | OD1 | ASN | B | 57 | 55.184 | 10.631 | 56.689 | 1.000 | 47.13 |
| ATOM | 2700 | ND2 | ASN | B | 57 | 56.334 | 10.662 | 54.780 | 1.000 | 33.73 |
| ATOM | 2701 | C   | ASN | B | 57 | 58.478 | 10.794 | 58.001 | 1.000 | 32.39 |
| ATOM | 2702 | O   | ASN | B | 57 | 59.628 | 10.706 | 57.573 | 1.000 | 32.15 |
| ATOM | 2703 | N   | GLN | B | 58 | 57.985 | 11.955 | 58.419 | 1.000 | 33.50 |

**FIGURE 58**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2704 | CA  | GLN | B | 58 | 58.765 | 13.190 | 58.281 | 1.000 | 32.36 |
| ATOM | 2705 | CB  | GLN | B | 58 | 57.838 | 14.389 | 58.063 | 1.000 | 31.34 |
| ATOM | 2706 | CG  | GLN | B | 58 | 57.016 | 14.302 | 56.782 | 1.000 | 22.41 |
| ATOM | 2707 | CD  | GLN | B | 58 | 55.700 | 15.058 | 56.891 | 1.000 | 23.88 |
| ATOM | 2708 | OE1 | GLN | B | 58 | 54.809 | 14.711 | 57.668 | 1.000 | 33.63 |
| ATOM | 2709 | NE2 | GLN | B | 58 | 55.545 | 16.114 | 56.113 | 1.000 | 22.62 |
| ATOM | 2710 | C   | GLN | B | 58 | 59.652 | 13.445 | 59.490 | 1.000 | 25.07 |
| ATOM | 2711 | O   | GLN | B | 58 | 59.327 | 13.045 | 60.608 | 1.000 | 29.18 |
| ATOM | 2712 | N   | SER | B | 59 | 60.773 | 14.121 | 59.261 | 1.000 | 17.59 |
| ATOM | 2713 | CA  | SER | B | 59 | 61.737 | 14.383 | 60.317 | 1.000 | 24.95 |
| ATOM | 2714 | CB  | SER | B | 59 | 63.157 | 14.310 | 59.752 | 1.000 | 30.84 |
| ATOM | 2715 | OG  | SER | B | 59 | 63.355 | 15.365 | 58.819 | 1.000 | 51.69 |
| ATOM | 2716 | C   | SER | B | 59 | 61.503 | 15.745 | 60.971 | 1.000 | 27.35 |
| ATOM | 2717 | O   | SER | B | 59 | 60.751 | 16.555 | 60.421 | 1.000 | 26.25 |
| ATOM | 2718 | N   | CYS | B | 60 | 62.142 | 15.962 | 62.108 | 1.000 | 20.52 |
| ATOM | 2719 | CA  | CYS | B | 60 | 62.088 | 17.174 | 62.901 | 1.000 | 25.62 |
| ATOM | 2720 | CB  | CYS | B | 60 | 61.291 | 16.938 | 64.187 | 1.000 | 32.28 |
| ATOM | 2721 | SG  | CYS | B | 60 | 59.563 | 16.490 | 63.935 | 1.000 | 44.06 |
| ATOM | 2722 | C   | CYS | B | 60 | 63.483 | 17.658 | 63.294 | 1.000 | 26.82 |
| ATOM | 2723 | O   | CYS | B | 60 | 63.697 | 17.986 | 64.466 | 1.000 | 32.10 |
| ATOM | 2724 | N   | ASP | B | 61 | 64.399 | 17.692 | 62.342 | 1.000 | 27.28 |
| ATOM | 2725 | CA  | ASP | B | 61 | 65.796 | 18.026 | 62.568 | 1.000 | 27.04 |
| ATOM | 2726 | CB  | ASP | B | 61 | 66.567 | 17.889 | 61.242 | 1.000 | 38.19 |
| ATOM | 2727 | CG  | ASP | B | 61 | 66.412 | 16.519 | 60.605 | 1.000 | 50.13 |
| ATOM | 2728 | OD1 | ASP | B | 61 | 66.494 | 15.504 | 61.335 | 1.000 | 46.12 |
| ATOM | 2729 | OD2 | ASP | B | 61 | 66.204 | 16.442 | 59.370 | 1.000 | 33.84 |
| ATOM | 2730 | C   | ASP | B | 61 | 66.010 | 19.431 | 63.103 | 1.000 | 25.10 |
| ATOM | 2731 | O   | ASP | B | 61 | 66.821 | 19.666 | 63.995 | 1.000 | 32.03 |
| ATOM | 2732 | N   | ILE | B | 62 | 65.315 | 20.420 | 62.536 | 1.000 | 31.05 |
| ATOM | 2733 | CA  | ILE | B | 62 | 65.582 | 21.807 | 62.924 | 1.000 | 30.27 |
| ATOM | 2734 | CB  | ILE | B | 62 | 64.816 | 22.824 | 62.061 | 1.000 | 30.17 |
| ATOM | 2735 | CG1 | ILE | B | 62 | 65.175 | 22.724 | 60.577 | 1.000 | 33.67 |
| ATOM | 2736 | CD1 | ILE | B | 62 | 66.676 | 22.691 | 60.345 | 1.000 | 39.64 |
| ATOM | 2737 | CG2 | ILE | B | 62 | 65.010 | 24.244 | 62.584 | 1.000 | 21.41 |
| ATOM | 2738 | C   | ILE | B | 62 | 65.202 | 22.019 | 64.382 | 1.000 | 32.48 |
| ATOM | 2739 | O   | ILE | B | 62 | 65.907 | 22.658 | 65.156 | 1.000 | 29.08 |
| ATOM | 2740 | N   | ALA | B | 63 | 64.048 | 21.444 | 64.738 | 1.000 | 26.00 |
| ATOM | 2741 | CA  | ALA | B | 63 | 63.649 | 21.631 | 66.136 | 1.000 | 26.52 |
| ATOM | 2742 | CB  | ALA | B | 63 | 62.232 | 21.116 | 66.313 | 1.000 | 16.06 |
| ATOM | 2743 | C   | ALA | B | 63 | 64.643 | 20.948 | 67.058 | 1.000 | 26.00 |
| ATOM | 2744 | O   | ALA | B | 63 | 64.789 | 21.266 | 68.235 | 1.000 | 32.44 |
| ATOM | 2745 | N   | LEU | B | 64 | 65.380 | 19.963 | 66.558 | 1.000 | 29.22 |
| ATOM | 2746 | CA  | LEU | B | 64 | 66.274 | 19.228 | 67.458 | 1.000 | 36.10 |
| ATOM | 2747 | CB  | LEU | B | 64 | 66.389 | 17.787 | 66.957 | 1.000 | 34.83 |
| ATOM | 2748 | CG  | LEU | B | 64 | 65.227 | 16.867 | 67.351 | 1.000 | 34.44 |
| ATOM | 2749 | CD1 | LEU | B | 64 | 65.292 | 15.577 | 66.547 | 1.000 | 29.17 |
| ATOM | 2750 | CD2 | LEU | B | 64 | 65.242 | 16.616 | 68.853 | 1.000 | 22.34 |
| ATOM | 2751 | C   | LEU | B | 64 | 67.641 | 19.880 | 67.584 | 1.000 | 38.72 |
| ATOM | 2752 | O   | LEU | B | 64 | 68.466 | 19.505 | 68.423 | 1.000 | 33.43 |
| ATOM | 2753 | N   | LEU | B | 65 | 67.910 | 20.882 | 66.752 | 1.000 | 29.69 |
| ATOM | 2754 | CA  | LEU | B | 65 | 69.194 | 21.567 | 66.816 | 1.000 | 24.50 |
| ATOM | 2755 | CB  | LEU | B | 65 | 69.248 | 22.693 | 65.788 | 1.000 | 23.85 |

**FIGURE 59**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2756 | CG  | LEU | B | 65 | 69.163 | 22.287 | 64.320 | 1.000 | 39.84 |
| ATOM | 2757 | CD1 | LEU | B | 65 | 68.898 | 23.516 | 63.459 | 1.000 | 38.18 |
| ATOM | 2758 | CD2 | LEU | B | 65 | 70.432 | 21.567 | 63.880 | 1.000 | 36.27 |
| ATOM | 2759 | C   | LEU | B | 65 | 69.438 | 22.122 | 68.218 | 1.000 | 36.38 |
| ATOM | 2760 | O   | LEU | B | 65 | 68.526 | 22.606 | 68.883 | 1.000 | 40.63 |
| ATOM | 2761 | N   | PRO | B | 66 | 70.686 | 22.026 | 68.657 | 1.000 | 45.15 |
| ATOM | 2762 | CA  | PRO | B | 66 | 71.066 | 22.422 | 70.011 | 1.000 | 54.26 |
| ATOM | 2763 | CB  | PRO | B | 66 | 72.601 | 22.452 | 69.931 | 1.000 | 52.68 |
| ATOM | 2764 | CG  | PRO | B | 66 | 72.910 | 21.394 | 68.918 | 1.000 | 46.70 |
| ATOM | 2765 | CD  | PRO | B | 66 | 71.831 | 21.512 | 67.881 | 1.000 | 44.93 |
| ATOM | 2766 | C   | PRO | B | 66 | 70.553 | 23.796 | 70.415 | 1.000 | 50.86 |
| ATOM | 2767 | O   | PRO | B | 66 | 70.105 | 23.966 | 71.552 | 1.000 | 48.53 |
| ATOM | 2768 | N   | GLU | B | 67 | 70.616 | 24.767 | 69.510 | 1.000 | 51.81 |
| ATOM | 2769 | CA  | GLU | B | 67 | 70.250 | 26.137 | 69.872 | 1.000 | 51.43 |
| ATOM | 2770 | CB  | GLU | B | 67 | 70.880 | 27.124 | 68.885 | 1.000 | 55.34 |
| ATOM | 2771 | CG  | GLU | B | 67 | 71.814 | 28.138 | 69.522 | 1.000 | 71.70 |
| ATOM | 2772 | CD  | GLU | B | 67 | 71.302 | 28.794 | 70.787 | 1.000 | 77.75 |
| ATOM | 2773 | OE1 | GLU | B | 67 | 72.110 | 28.959 | 71.733 | 1.000 | 81.38 |
| ATOM | 2774 | OE2 | GLU | B | 67 | 70.109 | 29.159 | 70.864 | 1.000 | 60.23 |
| ATOM | 2775 | C   | GLU | B | 67 | 68.745 | 26.354 | 69.938 | 1.000 | 46.00 |
| ATOM | 2776 | O   | GLU | B | 67 | 68.296 | 27.474 | 70.196 | 1.000 | 48.84 |
| ATOM | 2777 | N   | ASN | B | 68 | 67.944 | 25.314 | 69.711 | 1.000 | 40.69 |
| ATOM | 2778 | CA  | ASN | B | 68 | 66.494 | 25.487 | 69.755 | 1.000 | 36.03 |
| ATOM | 2779 | CB  | ASN | B | 68 | 65.825 | 24.980 | 68.477 | 1.000 | 39.69 |
| ATOM | 2780 | CG  | ASN | B | 68 | 66.147 | 25.780 | 67.233 | 1.000 | 33.61 |
| ATOM | 2781 | OD1 | ASN | B | 68 | 66.504 | 26.952 | 67.287 | 1.000 | 31.83 |
| ATOM | 2782 | ND2 | ASN | B | 68 | 66.038 | 25.160 | 66.060 | 1.000 | 31.89 |
| ATOM | 2783 | C   | ASN | B | 68 | 65.914 | 24.759 | 70.964 | 1.000 | 34.09 |
| ATOM | 2784 | O   | ASN | B | 68 | 64.719 | 24.859 | 71.235 | 1.000 | 47.57 |
| ATOM | 2785 | N   | ARG | B | 69 | 66.765 | 24.038 | 71.685 | 1.000 | 36.03 |
| ATOM | 2786 | CA  | ARG | B | 69 | 66.306 | 23.202 | 72.792 | 1.000 | 41.44 |
| ATOM | 2787 | CB  | ARG | B | 69 | 67.483 | 22.545 | 73.522 | 1.000 | 43.89 |
| ATOM | 2788 | CG  | ARG | B | 69 | 67.790 | 21.126 | 73.075 | 1.000 | 54.59 |
| ATOM | 2789 | CD  | ARG | B | 69 | 68.623 | 21.108 | 71.802 | 1.000 | 63.54 |
| ATOM | 2790 | NE  | ARG | B | 69 | 68.602 | 19.813 | 71.126 | 1.000 | 68.27 |
| ATOM | 2791 | CZ  | ARG | B | 69 | 69.645 | 18.999 | 71.016 | 1.000 | 73.48 |
| ATOM | 2792 | NH1 | ARG | B | 69 | 70.812 | 19.341 | 71.551 | 1.000 | 75.03 |
| ATOM | 2793 | NH2 | ARG | B | 69 | 69.536 | 17.838 | 70.378 | 1.000 | 71.51 |
| ATOM | 2794 | C   | ARG | B | 69 | 65.466 | 23.990 | 73.787 | 1.000 | 37.64 |
| ATOM | 2795 | O   | ARG | B | 69 | 64.448 | 23.486 | 74.260 | 1.000 | 47.56 |
| ATOM | 2796 | N   | GLY | B | 70 | 65.885 | 25.212 | 74.117 | 1.000 | 32.41 |
| ATOM | 2797 | CA  | GLY | B | 70 | 65.107 | 25.974 | 75.086 | 1.000 | 30.87 |
| ATOM | 2798 | C   | GLY | B | 70 | 63.789 | 26.425 | 74.495 | 1.000 | 31.35 |
| ATOM | 2799 | O   | GLY | B | 70 | 62.881 | 26.880 | 75.183 | 1.000 | 32.44 |
| ATOM | 2800 | N   | LYS | B | 71 | 63.642 | 26.301 | 73.172 | 1.000 | 28.40 |
| ATOM | 2801 | CA  | LYS | B | 71 | 62.431 | 26.876 | 72.579 | 1.000 | 23.17 |
| ATOM | 2802 | CB  | LYS | B | 71 | 62.809 | 27.437 | 71.205 | 1.000 | 24.12 |
| ATOM | 2803 | CG  | LYS | B | 71 | 63.920 | 28.476 | 71.318 | 1.000 | 25.57 |
| ATOM | 2804 | CD  | LYS | B | 71 | 64.674 | 28.583 | 70.010 | 1.000 | 30.17 |
| ATOM | 2805 | CE  | LYS | B | 71 | 65.580 | 29.802 | 69.994 | 1.000 | 37.46 |
| ATOM | 2806 | NZ  | LYS | B | 71 | 66.319 | 29.886 | 68.700 | 1.000 | 51.92 |
| ATOM | 2807 | C   | LYS | B | 71 | 61.296 | 25.876 | 72.492 | 1.000 | 23.16 |

**FIGURE 60**



Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2808 | O   | LYS | B | 71 | 60.205 | 26.158 | 71.995 | 1.000 | 27.70 |
| ATOM | 2809 | N   | ASN | B | 72 | 61.501 | 24.663 | 72.997 | 1.000 | 19.21 |
| ATOM | 2810 | CA  | ASN | B | 72 | 60.414 | 23.691 | 72.972 | 1.000 | 21.63 |
| ATOM | 2811 | CB  | ASN | B | 72 | 60.918 | 22.370 | 72.375 | 1.000 | 26.16 |
| ATOM | 2812 | CG  | ASN | B | 72 | 61.306 | 22.543 | 70.916 | 1.000 | 31.09 |
| ATOM | 2813 | OD1 | ASN | B | 72 | 60.465 | 22.945 | 70.109 | 1.000 | 26.04 |
| ATOM | 2814 | ND2 | ASN | B | 72 | 62.558 | 22.245 | 70.577 | 1.000 | 24.16 |
| ATOM | 2815 | C   | ASN | B | 72 | 59.855 | 23.481 | 74.369 | 1.000 | 28.90 |
| ATOM | 2816 | O   | ASN | B | 72 | 60.603 | 23.340 | 75.333 | 1.000 | 27.09 |
| ATOM | 2817 | N   | ARG | B | 73 | 58.532 | 23.462 | 74.504 | 1.000 | 29.94 |
| ATOM | 2818 | CA  | ARG | B | 73 | 57.950 | 23.251 | 75.827 | 1.000 | 29.94 |
| ATOM | 2819 | CB  | ARG | B | 73 | 56.501 | 23.738 | 75.862 | 1.000 | 30.13 |
| ATOM | 2820 | CG  | ARG | B | 73 | 55.847 | 23.665 | 77.239 | 1.000 | 26.45 |
| ATOM | 2821 | CD  | ARG | B | 73 | 54.393 | 24.129 | 77.156 | 1.000 | 21.48 |
| ATOM | 2822 | NE  | ARG | B | 73 | 54.347 | 25.597 | 77.101 | 1.000 | 21.98 |
| ATOM | 2823 | CZ  | ARG | B | 73 | 54.413 | 26.305 | 78.225 | 1.000 | 30.47 |
| ATOM | 2824 | NH1 | ARG | B | 73 | 54.514 | 25.676 | 79.390 | 1.000 | 22.83 |
| ATOM | 2825 | NH2 | ARG | B | 73 | 54.373 | 27.624 | 78.162 | 1.000 | 37.96 |
| ATOM | 2826 | C   | ARG | B | 73 | 58.047 | 21.775 | 76.205 | 1.000 | 36.82 |
| ATOM | 2827 | O   | ARG | B | 73 | 58.212 | 21.428 | 77.375 | 1.000 | 27.47 |
| ATOM | 2828 | N   | TYR | B | 74 | 57.948 | 20.904 | 75.202 | 1.000 | 27.29 |
| ATOM | 2829 | CA  | TYR | B | 74 | 58.101 | 19.470 | 75.416 | 1.000 | 24.94 |
| ATOM | 2830 | CB  | TYR | B | 74 | 56.774 | 18.731 | 75.335 | 1.000 | 24.22 |
| ATOM | 2831 | CG  | TYR | B | 74 | 55.661 | 19.265 | 76.209 | 1.000 | 31.66 |
| ATOM | 2832 | CD1 | TYR | B | 74 | 55.531 | 18.876 | 77.540 | 1.000 | 37.63 |
| ATOM | 2833 | CE1 | TYR | B | 74 | 54.513 | 19.366 | 78.342 | 1.000 | 39.66 |
| ATOM | 2834 | CZ  | TYR | B | 74 | 53.601 | 20.258 | 77.818 | 1.000 | 38.75 |
| ATOM | 2835 | OH  | TYR | B | 74 | 52.588 | 20.745 | 78.608 | 1.000 | 34.40 |
| ATOM | 2836 | CE2 | TYR | B | 74 | 53.695 | 20.668 | 76.503 | 1.000 | 25.62 |
| ATOM | 2837 | CD2 | TYR | B | 74 | 54.722 | 20.163 | 75.724 | 1.000 | 27.42 |
| ATOM | 2838 | C   | TYR | B | 74 | 59.091 | 18.944 | 74.377 | 1.000 | 34.07 |
| ATOM | 2839 | O   | TYR | B | 74 | 58.878 | 19.078 | 73.170 | 1.000 | 35.65 |
| ATOM | 2840 | N   | ASN | B | 75 | 60.170 | 18.362 | 74.871 | 1.000 | 32.88 |
| ATOM | 2841 | CA  | ASN | B | 75 | 61.260 | 17.890 | 74.027 | 1.000 | 35.16 |
| ATOM | 2842 | CB  | ASN | B | 75 | 62.397 | 17.415 | 74.942 | 1.000 | 41.15 |
| ATOM | 2843 | CG  | ASN | B | 75 | 63.227 | 18.582 | 75.448 | 1.000 | 49.51 |
| ATOM | 2844 | OD1 | ASN | B | 75 | 64.296 | 18.392 | 76.032 | 1.000 | 62.29 |
| ATOM | 2845 | ND2 | ASN | B | 75 | 62.756 | 19.808 | 75.230 | 1.000 | 47.01 |
| ATOM | 2846 | C   | ASN | B | 75 | 60.832 | 16.813 | 73.042 | 1.000 | 27.77 |
| ATOM | 2847 | O   | ASN | B | 75 | 61.544 | 16.541 | 72.062 | 1.000 | 31.84 |
| ATOM | 2848 | N   | ASN | B | 76 | 59.676 | 16.191 | 73.248 | 1.000 | 24.48 |
| ATOM | 2849 | CA  | ASN | B | 76 | 59.194 | 15.180 | 72.303 | 1.000 | 31.98 |
| ATOM | 2850 | CB  | ASN | B | 76 | 58.888 | 13.857 | 73.026 | 1.000 | 39.45 |
| ATOM | 2851 | CG  | ASN | B | 76 | 57.794 | 14.002 | 74.065 | 1.000 | 36.56 |
| ATOM | 2852 | OD1 | ASN | B | 76 | 57.640 | 15.076 | 74.643 | 1.000 | 29.01 |
| ATOM | 2853 | ND2 | ASN | B | 76 | 57.038 | 12.939 | 74.311 | 1.000 | 28.69 |
| ATOM | 2854 | C   | ASN | B | 76 | 57.964 | 15.646 | 71.535 | 1.000 | 35.01 |
| ATOM | 2855 | O   | ASN | B | 76 | 57.304 | 14.845 | 70.863 | 1.000 | 26.16 |
| ATOM | 2856 | N   | ILE | B | 77 | 57.641 | 16.943 | 71.608 | 1.000 | 28.11 |
| ATOM | 2857 | CA  | ILE | B | 77 | 56.567 | 17.443 | 70.743 | 1.000 | 30.83 |
| ATOM | 2858 | CB  | ILE | B | 77 | 55.318 | 17.839 | 71.534 | 1.000 | 30.03 |
| ATOM | 2859 | CG1 | ILE | B | 77 | 54.547 | 16.646 | 72.114 | 1.000 | 33.86 |

**FIGURE 61**

|      |      |     |     |   |    |        |        |        |       |       |
|------|------|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 2860 | CD1 | ILE | B | 77 | 53.956 | 16.931 | 73.479 | 1.000 | 23.65 |
| ATOM | 2861 | CG2 | ILE | B | 77 | 54.400 | 18.697 | 70.690 | 1.000 | 34.46 |
| ATOM | 2862 | C   | ILE | B | 77 | 57.078 | 18.622 | 69.914 | 1.000 | 27.23 |
| ATOM | 2863 | O   | ILE | B | 77 | 57.193 | 19.748 | 70.388 | 1.000 | 22.76 |
| ATOM | 2864 | N   | LEU | B | 78 | 57.404 | 18.308 | 68.668 | 1.000 | 23.21 |
| ATOM | 2865 | CA  | LEU | B | 78 | 58.101 | 19.170 | 67.741 | 1.000 | 24.29 |
| ATOM | 2866 | CB  | LEU | B | 78 | 59.571 | 18.763 | 67.579 | 1.000 | 30.93 |
| ATOM | 2867 | CG  | LEU | B | 78 | 60.317 | 18.344 | 68.845 | 1.000 | 29.39 |
| ATOM | 2868 | CD1 | LEU | B | 78 | 61.596 | 17.606 | 68.496 | 1.000 | 30.84 |
| ATOM | 2869 | CD2 | LEU | B | 78 | 60.606 | 19.563 | 69.702 | 1.000 | 39.96 |
| ATOM | 2870 | C   | LEU | B | 78 | 57.477 | 19.158 | 66.348 | 1.000 | 27.34 |
| ATOM | 2871 | O   | LEU | B | 78 | 56.883 | 18.186 | 65.883 | 1.000 | 22.52 |
| ATOM | 2872 | N   | PRO | B | 79 | 57.653 | 20.300 | 65.695 | 1.000 | 26.68 |
| ATOM | 2873 | CA  | PRO | B | 79 | 57.097 | 20.468 | 64.351 | 1.000 | 19.33 |
| ATOM | 2874 | CB  | PRO | B | 79 | 57.244 | 21.974 | 64.135 | 1.000 | 20.00 |
| ATOM | 2875 | CG  | PRO | B | 79 | 58.491 | 22.309 | 64.892 | 1.000 | 17.51 |
| ATOM | 2876 | CD  | PRO | B | 79 | 58.384 | 21.490 | 66.156 | 1.000 | 17.54 |
| ATOM | 2877 | C   | PRO | B | 79 | 57.939 | 19.691 | 63.351 | 1.000 | 18.83 |
| ATOM | 2878 | O   | PRO | B | 79 | 59.161 | 19.657 | 63.510 | 1.000 | 24.06 |
| ATOM | 2879 | N   | TYR | B | 80 | 57.287 | 19.098 | 62.367 | 1.000 | 18.71 |
| ATOM | 2880 | CA  | TYR | B | 80 | 57.911 | 18.548 | 61.181 | 1.000 | 17.89 |
| ATOM | 2881 | CB  | TYR | B | 80 | 56.857 | 17.886 | 60.297 | 1.000 | 30.40 |
| ATOM | 2882 | CG  | TYR | B | 80 | 56.167 | 16.688 | 60.900 | 1.000 | 29.81 |
| ATOM | 2883 | CD1 | TYR | B | 80 | 56.876 | 15.711 | 61.589 | 1.000 | 27.11 |
| ATOM | 2884 | CE1 | TYR | B | 80 | 56.247 | 14.607 | 62.147 | 1.000 | 26.90 |
| ATOM | 2885 | CZ  | TYR | B | 80 | 54.885 | 14.478 | 62.004 | 1.000 | 27.92 |
| ATOM | 2886 | OH  | TYR | B | 80 | 54.233 | 13.393 | 62.539 | 1.000 | 22.86 |
| ATOM | 2887 | CE2 | TYR | B | 80 | 54.162 | 15.432 | 61.324 | 1.000 | 21.67 |
| ATOM | 2888 | CD2 | TYR | B | 80 | 54.794 | 16.532 | 60.774 | 1.000 | 22.55 |
| ATOM | 2889 | C   | TYR | B | 80 | 58.600 | 19.647 | 60.373 | 1.000 | 26.95 |
| ATOM | 2890 | O   | TYR | B | 80 | 58.000 | 20.703 | 60.137 | 1.000 | 29.85 |
| ATOM | 2891 | N   | ASP | B | 81 | 59.836 | 19.401 | 59.962 | 1.000 | 23.42 |
| ATOM | 2892 | CA  | ASP | B | 81 | 60.607 | 20.320 | 59.148 | 1.000 | 23.41 |
| ATOM | 2893 | CB  | ASP | B | 81 | 61.878 | 19.642 | 58.613 | 1.000 | 34.98 |
| ATOM | 2894 | CG  | ASP | B | 81 | 62.914 | 19.322 | 59.664 | 1.000 | 32.41 |
| ATOM | 2895 | OD1 | ASP | B | 81 | 62.951 | 20.053 | 60.680 | 1.000 | 35.92 |
| ATOM | 2896 | OD2 | ASP | B | 81 | 63.686 | 18.346 | 59.510 | 1.000 | 30.60 |
| ATOM | 2897 | C   | ASP | B | 81 | 59.795 | 20.828 | 57.959 | 1.000 | 25.69 |
| ATOM | 2898 | O   | ASP | B | 81 | 59.760 | 22.011 | 57.634 | 1.000 | 33.08 |
| ATOM | 2899 | N   | ALA | B | 82 | 59.122 | 19.915 | 57.268 | 1.000 | 28.44 |
| ATOM | 2900 | CA  | ALA | B | 82 | 58.455 | 20.249 | 56.015 | 1.000 | 30.21 |
| ATOM | 2901 | CB  | ALA | B | 82 | 57.984 | 18.939 | 55.373 | 1.000 | 26.10 |
| ATOM | 2902 | C   | ALA | B | 82 | 57.283 | 21.200 | 56.164 | 1.000 | 29.54 |
| ATOM | 2903 | O   | ALA | B | 82 | 56.790 | 21.814 | 55.211 | 1.000 | 25.55 |
| ATOM | 2904 | N   | THR | B | 83 | 56.753 | 21.363 | 57.372 | 1.000 | 22.96 |
| ATOM | 2905 | CA  | THR | B | 83 | 55.542 | 22.170 | 57.495 | 1.000 | 22.68 |
| ATOM | 2906 | CB  | THR | B | 83 | 54.342 | 21.270 | 57.845 | 1.000 | 29.40 |
| ATOM | 2907 | OG1 | THR | B | 83 | 54.667 | 20.507 | 59.014 | 1.000 | 20.17 |
| ATOM | 2908 | CG2 | THR | B | 83 | 54.087 | 20.287 | 56.713 | 1.000 | 25.89 |
| ATOM | 2909 | C   | THR | B | 83 | 55.677 | 23.231 | 58.566 | 1.000 | 23.50 |
| ATOM | 2910 | O   | THR | B | 83 | 54.681 | 23.841 | 58.936 | 1.000 | 22.92 |
| ATOM | 2911 | N   | ARG | B | 84 | 56.897 | 23.443 | 59.056 | 1.000 | 25.87 |

**FIGURE 62**

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|      |      |     |     |   |    |        |        |        |       |        |
|------|------|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 2912 | CA  | ARG | B | 84 | 57.050 | 24.372 | 60.171 | 1.000 | 26.66  |
| ATOM | 2913 | CB  | ARG | B | 84 | 58.405 | 24.149 | 60.862 | 1.000 | 26.13  |
| ATOM | 2914 | CG  | ARG | B | 84 | 59.618 | 24.541 | 60.040 | 1.000 | 22.35  |
| ATOM | 2915 | CD  | ARG | B | 84 | 60.929 | 24.294 | 60.779 | 1.000 | 26.61  |
| ATOM | 2916 | NE  | ARG | B | 84 | 62.018 | 24.933 | 60.053 | 1.000 | 28.50  |
| ATOM | 2917 | CZ  | ARG | B | 84 | 62.683 | 26.031 | 60.352 | 1.000 | 29.24  |
| ATOM | 2918 | NH1 | ARG | B | 84 | 62.442 | 26.754 | 61.435 | 1.000 | 24.43  |
| ATOM | 2919 | NH2 | ARG | B | 84 | 63.645 | 26.433 | 59.530 | 1.000 | 32.59  |
| ATOM | 2920 | C   | ARG | B | 84 | 56.890 | 25.819 | 59.728 | 1.000 | 22.30  |
| ATOM | 2921 | O   | ARG | B | 84 | 57.133 | 26.183 | 58.583 | 1.000 | 23.04  |
| ATOM | 2922 | N   | VAL | B | 85 | 56.477 | 26.663 | 60.669 | 1.000 | 18.94  |
| ATOM | 2923 | CA  | VAL | B | 85 | 56.405 | 28.101 | 60.424 | 1.000 | 21.51  |
| ATOM | 2924 | CB  | VAL | B | 85 | 55.322 | 28.738 | 61.308 | 1.000 | 18.95  |
| ATOM | 2925 | CG1 | VAL | B | 85 | 55.256 | 30.249 | 61.152 | 1.000 | 24.35  |
| ATOM | 2926 | CG2 | VAL | B | 85 | 53.967 | 28.113 | 60.988 | 1.000 | 12.73  |
| ATOM | 2927 | C   | VAL | B | 85 | 57.776 | 28.707 | 60.699 | 1.000 | 25.23  |
| ATOM | 2928 | O   | VAL | B | 85 | 58.331 | 28.435 | 61.767 | 1.000 | 27.46  |
| ATOM | 2929 | N   | LYS | B | 86 | 58.320 | 29.488 | 59.782 | 1.000 | 19.69  |
| ATOM | 2930 | CA  | LYS | B | 86 | 59.624 | 30.120 | 59.878 | 1.000 | 21.25  |
| ATOM | 2931 | CB  | LYS | B | 86 | 60.321 | 30.044 | 58.509 | 1.000 | 26.66  |
| ATOM | 2932 | CG  | LYS | B | 86 | 60.905 | 28.675 | 58.194 | 1.000 | 33.26  |
| ATOM | 2933 | CD  | LYS | B | 86 | 60.950 | 28.412 | 56.698 | 1.000 | 34.06  |
| ATOM | 2934 | CE  | LYS | B | 86 | 61.685 | 27.121 | 56.377 | 1.000 | 41.77  |
| ATOM | 2935 | NZ  | LYS | B | 86 | 63.000 | 27.368 | 55.715 | 1.000 | 51.25  |
| ATOM | 2936 | C   | LYS | B | 86 | 59.558 | 31.584 | 60.289 | 1.000 | 27.93  |
| ATOM | 2937 | O   | LYS | B | 86 | 58.723 | 32.338 | 59.780 | 1.000 | 31.79  |
| ATOM | 2938 | N   | LEU | B | 87 | 60.431 | 32.027 | 61.194 | 1.000 | 31.15  |
| ATOM | 2939 | CA  | LEU | B | 87 | 60.507 | 33.457 | 61.505 | 1.000 | 28.89  |
| ATOM | 2940 | CB  | LEU | B | 87 | 61.126 | 33.736 | 62.870 | 1.000 | 21.77  |
| ATOM | 2941 | CG  | LEU | B | 87 | 60.472 | 33.041 | 64.066 | 1.000 | 30.37  |
| ATOM | 2942 | CD1 | LEU | B | 87 | 61.312 | 33.206 | 65.321 | 1.000 | 35.12  |
| ATOM | 2943 | CD2 | LEU | B | 87 | 59.066 | 33.577 | 64.279 | 1.000 | 22.71  |
| ATOM | 2944 | C   | LEU | B | 87 | 61.332 | 34.163 | 60.429 | 1.000 | 37.83  |
| ATOM | 2945 | O   | LEU | B | 87 | 62.297 | 33.589 | 59.913 | 1.000 | 30.13  |
| ATOM | 2946 | N   | SER | B | 88 | 60.944 | 35.389 | 60.100 | 1.000 | 36.67  |
| ATOM | 2947 | CA  | SER | B | 88 | 61.678 | 36.147 | 59.095 | 1.000 | 40.88  |
| ATOM | 2948 | CB  | SER | B | 88 | 61.145 | 37.572 | 58.969 | 1.000 | 50.96  |
| ATOM | 2949 | OG  | SER | B | 88 | 61.924 | 38.447 | 59.787 | 1.000 | 71.49  |
| ATOM | 2950 | C   | SER | B | 88 | 63.162 | 36.209 | 59.453 | 1.000 | 53.58  |
| ATOM | 2951 | O   | SER | B | 88 | 63.487 | 36.614 | 60.569 | 1.000 | 59.70  |
| ATOM | 2952 | N   | ASN | B | 89 | 63.971 | 35.800 | 58.503 | 1.000 | 71.44  |
| ATOM | 2953 | CA  | ASN | B | 89 | 65.419 | 35.723 | 58.486 | 1.000 | 85.86  |
| ATOM | 2954 | CB  | ASN | B | 89 | 65.871 | 36.099 | 57.064 | 1.000 | 85.53  |
| ATOM | 2955 | CG  | ASN | B | 89 | 64.906 | 35.515 | 56.046 | 1.000 | 83.74  |
| ATOM | 2956 | OD1 | ASN | B | 89 | 63.714 | 35.820 | 56.022 | 1.000 | 58.06  |
| ATOM | 2957 | ND2 | ASN | B | 89 | 65.435 | 34.646 | 55.196 | 1.000 | 94.70  |
| ATOM | 2958 | C   | ASN | B | 89 | 66.085 | 36.608 | 59.532 | 1.000 | 95.53  |
| ATOM | 2959 | O   | ASN | B | 89 | 66.500 | 37.726 | 59.230 | 1.000 | 106.63 |
| ATOM | 2960 | N   | VAL | B | 90 | 66.182 | 36.108 | 60.760 | 1.000 | 99.91  |
| ATOM | 2961 | CA  | VAL | B | 90 | 66.604 | 36.863 | 61.925 | 1.000 | 106.49 |
| ATOM | 2962 | CB  | VAL | B | 90 | 65.922 | 36.329 | 63.208 | 1.000 | 100.23 |
| ATOM | 2963 | CG1 | VAL | B | 90 | 65.594 | 37.484 | 64.140 | 1.000 | 85.61  |

**FIGURE 63**

|      |      |     |     |   |    |        |        |        |       |        |
|------|------|-----|-----|---|----|--------|--------|--------|-------|--------|
| ATOM | 2964 | CG2 | VAL | B | 90 | 64.673 | 35.536 | 62.861 | 1.000 | 93.25  |
| ATOM | 2965 | C   | VAL | B | 90 | 68.114 | 36.866 | 62.182 | 1.000 | 113.45 |
| ATOM | 2966 | O   | VAL | B | 90 | 68.832 | 35.943 | 61.806 | 1.000 | 122.31 |
| ATOM | 2967 | N   | ASP | B | 91 | 68.544 | 37.933 | 62.844 | 1.000 | 114.27 |
| ATOM | 2968 | CA  | ASP | B | 91 | 69.897 | 38.277 | 63.228 | 1.000 | 110.66 |
| ATOM | 2969 | CB  | ASP | B | 91 | 69.892 | 39.409 | 64.264 | 1.000 | 111.15 |
| ATOM | 2970 | CG  | ASP | B | 91 | 71.270 | 40.014 | 64.465 | 1.000 | 110.08 |
| ATOM | 2971 | OD1 | ASP | B | 91 | 71.763 | 40.698 | 63.539 | 1.000 | 108.01 |
| ATOM | 2972 | OD2 | ASP | B | 91 | 71.864 | 39.800 | 65.540 | 1.000 | 107.80 |
| ATOM | 2973 | C   | ASP | B | 91 | 70.667 | 37.090 | 63.802 | 1.000 | 103.90 |
| ATOM | 2974 | O   | ASP | B | 91 | 70.062 | 36.112 | 64.251 | 1.000 | 107.40 |
| ATOM | 2975 | N   | ASP | B | 92 | 71.989 | 37.191 | 63.769 | 1.000 | 95.56  |
| ATOM | 2976 | CA  | ASP | B | 92 | 72.913 | 36.160 | 64.216 | 1.000 | 92.84  |
| ATOM | 2977 | CB  | ASP | B | 92 | 72.475 | 35.573 | 65.557 | 1.000 | 96.48  |
| ATOM | 2978 | CG  | ASP | B | 92 | 73.473 | 35.776 | 66.676 | 1.000 | 98.09  |
| ATOM | 2979 | OD1 | ASP | B | 92 | 73.609 | 34.872 | 67.529 | 1.000 | 84.88  |
| ATOM | 2980 | OD2 | ASP | B | 92 | 74.122 | 36.837 | 66.715 | 1.000 | 107.58 |
| ATOM | 2981 | C   | ASP | B | 92 | 73.036 | 35.057 | 63.161 | 1.000 | 91.94  |
| ATOM | 2982 | O   | ASP | B | 92 | 74.144 | 34.632 | 62.832 | 1.000 | 94.07  |
| ATOM | 2983 | N   | ASP | B | 93 | 71.901 | 34.619 | 62.650 | 1.000 | 91.73  |
| ATOM | 2984 | CA  | ASP | B | 93 | 71.682 | 33.642 | 61.611 | 1.000 | 95.04  |
| ATOM | 2985 | CB  | ASP | B | 93 | 72.393 | 34.073 | 60.319 | 1.000 | 103.17 |
| ATOM | 2986 | CG  | ASP | B | 93 | 71.728 | 35.227 | 59.594 | 1.000 | 106.58 |
| ATOM | 2987 | OD1 | ASP | B | 93 | 70.954 | 34.993 | 58.638 | 1.000 | 104.63 |
| ATOM | 2988 | OD2 | ASP | B | 93 | 71.988 | 36.396 | 59.962 | 1.000 | 107.25 |
| ATOM | 2989 | C   | ASP | B | 93 | 72.140 | 32.243 | 62.001 | 1.000 | 91.99  |
| ATOM | 2990 | O   | ASP | B | 93 | 72.871 | 31.598 | 61.239 | 1.000 | 105.20 |
| ATOM | 2991 | N   | PRO | B | 94 | 71.753 | 31.714 | 63.147 | 1.000 | 86.76  |
| ATOM | 2992 | CA  | PRO | B | 94 | 72.111 | 30.328 | 63.491 | 1.000 | 84.05  |
| ATOM | 2993 | CB  | PRO | B | 94 | 72.346 | 30.431 | 64.992 | 1.000 | 81.07  |
| ATOM | 2994 | CG  | PRO | B | 94 | 71.549 | 31.600 | 65.461 | 1.000 | 79.07  |
| ATOM | 2995 | CD  | PRO | B | 94 | 70.967 | 32.274 | 64.262 | 1.000 | 82.73  |
| ATOM | 2996 | C   | PRO | B | 94 | 70.930 | 29.403 | 63.184 | 1.000 | 88.17  |
| ATOM | 2997 | O   | PRO | B | 94 | 70.886 | 28.767 | 62.140 | 1.000 | 95.17  |
| ATOM | 2998 | N   | CYS | B | 95 | 70.014 | 29.396 | 64.129 | 1.000 | 85.15  |
| ATOM | 2999 | CA  | CYS | B | 95 | 68.692 | 28.806 | 64.171 | 1.000 | 71.00  |
| ATOM | 3000 | CB  | CYS | B | 95 | 68.676 | 27.559 | 65.048 | 1.000 | 68.25  |
| ATOM | 3001 | SG  | CYS | B | 95 | 70.324 | 27.048 | 65.606 | 1.000 | 59.08  |
| ATOM | 3002 | C   | CYS | B | 95 | 67.724 | 29.872 | 64.691 | 1.000 | 61.59  |
| ATOM | 3003 | O   | CYS | B | 95 | 66.839 | 29.638 | 65.507 | 1.000 | 45.14  |
| ATOM | 3004 | N   | SER | B | 96 | 67.966 | 31.077 | 64.176 | 1.000 | 54.56  |
| ATOM | 3005 | CA  | SER | B | 96 | 67.227 | 32.262 | 64.582 | 1.000 | 54.51  |
| ATOM | 3006 | CB  | SER | B | 96 | 67.962 | 33.527 | 64.131 | 1.000 | 53.89  |
| ATOM | 3007 | OG  | SER | B | 96 | 68.750 | 33.268 | 62.979 | 1.000 | 64.41  |
| ATOM | 3008 | C   | SER | B | 96 | 65.806 | 32.239 | 64.029 | 1.000 | 47.05  |
| ATOM | 3009 | O   | SER | B | 96 | 64.946 | 32.971 | 64.526 | 1.000 | 50.88  |
| ATOM | 3010 | N   | ASP | B | 97 | 65.565 | 31.402 | 63.024 | 1.000 | 36.23  |
| ATOM | 3011 | CA  | ASP | B | 97 | 64.263 | 31.360 | 62.369 | 1.000 | 27.85  |
| ATOM | 3012 | CB  | ASP | B | 97 | 64.461 | 30.914 | 60.911 | 1.000 | 24.26  |
| ATOM | 3013 | CG  | ASP | B | 97 | 64.720 | 29.419 | 60.834 | 1.000 | 36.82  |
| ATOM | 3014 | OD1 | ASP | B | 97 | 65.206 | 28.822 | 61.819 | 1.000 | 38.88  |
| ATOM | 3015 | OD2 | ASP | B | 97 | 64.431 | 28.828 | 59.772 | 1.000 | 52.38  |

**FIGURE 64**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3016 | C   | ASP | B | 97  | 63.263 | 30.420 | 63.027 | 1.000 | 29.64 |
| ATOM | 3017 | O   | ASP | B | 97  | 62.132 | 30.313 | 62.537 | 1.000 | 25.93 |
| ATOM | 3018 | N   | TYR | B | 98  | 63.653 | 29.727 | 64.094 | 1.000 | 31.48 |
| ATOM | 3019 | CA  | TYR | B | 98  | 62.830 | 28.686 | 64.683 | 1.000 | 27.28 |
| ATOM | 3020 | CB  | TYR | B | 98  | 63.708 | 27.639 | 65.426 | 1.000 | 24.83 |
| ATOM | 3021 | CG  | TYR | B | 98  | 62.860 | 26.500 | 65.960 | 1.000 | 19.17 |
| ATOM | 3022 | CD1 | TYR | B | 98  | 62.365 | 25.535 | 65.080 | 1.000 | 20.66 |
| ATOM | 3023 | CE1 | TYR | B | 98  | 61.587 | 24.485 | 65.523 | 1.000 | 24.11 |
| ATOM | 3024 | CZ  | TYR | B | 98  | 61.285 | 24.380 | 66.864 | 1.000 | 26.77 |
| ATOM | 3025 | OH  | TYR | B | 98  | 60.508 | 23.331 | 67.317 | 1.000 | 19.75 |
| ATOM | 3026 | CE2 | TYR | B | 98  | 61.760 | 25.324 | 67.751 | 1.000 | 22.13 |
| ATOM | 3027 | CD2 | TYR | B | 98  | 62.540 | 26.372 | 67.306 | 1.000 | 20.85 |
| ATOM | 3028 | C   | TYR | B | 98  | 61.775 | 29.132 | 65.687 | 1.000 | 20.04 |
| ATOM | 3029 | O   | TYR | B | 98  | 61.972 | 29.920 | 66.608 | 1.000 | 25.66 |
| ATOM | 3030 | N   | ILE | B | 99  | 60.604 | 28.517 | 65.531 | 1.000 | 20.57 |
| ATOM | 3031 | CA  | ILE | B | 99  | 59.546 | 28.552 | 66.532 | 1.000 | 19.42 |
| ATOM | 3032 | CB  | ILE | B | 99  | 58.577 | 29.720 | 66.314 | 1.000 | 19.96 |
| ATOM | 3033 | CG1 | ILE | B | 99  | 57.447 | 29.790 | 67.336 | 1.000 | 17.02 |
| ATOM | 3034 | CD1 | ILE | B | 99  | 56.771 | 31.140 | 67.413 | 1.000 | 19.58 |
| ATOM | 3035 | CG2 | ILE | B | 99  | 58.013 | 29.694 | 64.897 | 1.000 | 29.56 |
| ATOM | 3036 | C   | ILE | B | 99  | 58.773 | 27.240 | 66.500 | 1.000 | 22.92 |
| ATOM | 3037 | O   | ILE | B | 99  | 58.543 | 26.677 | 65.428 | 1.000 | 23.59 |
| ATOM | 3038 | N   | ASN | B | 100 | 58.373 | 26.722 | 67.665 | 1.000 | 17.01 |
| ATOM | 3039 | CA  | ASN | B | 100 | 57.617 | 25.462 | 67.617 | 1.000 | 20.62 |
| ATOM | 3040 | CB  | ASN | B | 100 | 57.574 | 24.797 | 68.989 | 1.000 | 22.98 |
| ATOM | 3041 | CG  | ASN | B | 100 | 56.990 | 23.404 | 68.998 | 1.000 | 24.77 |
| ATOM | 3042 | OD1 | ASN | B | 100 | 56.001 | 23.116 | 68.319 | 1.000 | 25.34 |
| ATOM | 3043 | ND2 | ASN | B | 100 | 57.571 | 22.496 | 69.786 | 1.000 | 18.32 |
| ATOM | 3044 | C   | ASN | B | 100 | 56.226 | 25.777 | 67.081 | 1.000 | 20.30 |
| ATOM | 3045 | O   | ASN | B | 100 | 55.361 | 26.152 | 67.888 | 1.000 | 19.79 |
| ATOM | 3046 | N   | ALA | B | 101 | 56.067 | 25.654 | 65.760 | 1.000 | 21.42 |
| ATOM | 3047 | CA  | ALA | B | 101 | 54.782 | 25.946 | 65.121 | 1.000 | 21.68 |
| ATOM | 3048 | CB  | ALA | B | 101 | 54.559 | 27.450 | 65.071 | 1.000 | 13.80 |
| ATOM | 3049 | C   | ALA | B | 101 | 54.696 | 25.326 | 63.732 | 1.000 | 26.20 |
| ATOM | 3050 | O   | ALA | B | 101 | 55.715 | 25.142 | 63.072 | 1.000 | 18.76 |
| ATOM | 3051 | N   | SER | B | 102 | 53.499 | 24.985 | 63.271 | 1.000 | 29.48 |
| ATOM | 3052 | CA  | SER | B | 102 | 53.250 | 24.285 | 62.023 | 1.000 | 19.07 |
| ATOM | 3053 | CB  | SER | B | 102 | 52.919 | 22.808 | 62.271 | 1.000 | 15.75 |
| ATOM | 3054 | OG  | SER | B | 102 | 53.753 | 22.258 | 63.274 | 1.000 | 21.52 |
| ATOM | 3055 | C   | SER | B | 102 | 52.073 | 24.879 | 61.259 | 1.000 | 19.78 |
| ATOM | 3056 | O   | SER | B | 102 | 51.068 | 25.227 | 61.882 | 1.000 | 21.21 |
| ATOM | 3057 | N   | TYR | B | 103 | 52.181 | 24.977 | 59.931 | 1.000 | 17.66 |
| ATOM | 3058 | CA  | TYR | B | 103 | 51.017 | 25.426 | 59.166 | 1.000 | 18.10 |
| ATOM | 3059 | CB  | TYR | B | 103 | 51.373 | 25.982 | 57.794 | 1.000 | 20.23 |
| ATOM | 3060 | CG  | TYR | B | 103 | 52.221 | 27.216 | 57.690 | 1.000 | 18.78 |
| ATOM | 3061 | CD1 | TYR | B | 103 | 51.692 | 28.498 | 57.841 | 1.000 | 22.17 |
| ATOM | 3062 | CE1 | TYR | B | 103 | 52.490 | 29.627 | 57.736 | 1.000 | 21.36 |
| ATOM | 3063 | CZ  | TYR | B | 103 | 53.840 | 29.489 | 57.472 | 1.000 | 23.55 |
| ATOM | 3064 | OH  | TYR | B | 103 | 54.656 | 30.597 | 57.367 | 1.000 | 21.98 |
| ATOM | 3065 | CE2 | TYR | B | 103 | 54.394 | 28.237 | 57.316 | 1.000 | 20.92 |
| ATOM | 3066 | CD2 | TYR | B | 103 | 53.585 | 27.113 | 57.422 | 1.000 | 26.09 |
| ATOM | 3067 | C   | TYR | B | 103 | 50.054 | 24.256 | 58.995 | 1.000 | 16.67 |

**FIGURE 65**

|      |      |     |           |        |        |        |       |       |
|------|------|-----|-----------|--------|--------|--------|-------|-------|
| ATOM | 3068 | O   | TYR B 103 | 50.489 | 23.126 | 58.760 | 1.000 | 22.66 |
| ATOM | 3069 | N   | ILE B 104 | 48.756 | 24.521 | 59.088 | 1.000 | 19.23 |
| ATOM | 3070 | CA  | ILE B 104 | 47.781 | 23.448 | 58.955 | 1.000 | 24.34 |
| ATOM | 3071 | CB  | ILE B 104 | 47.099 | 23.127 | 60.304 | 1.000 | 32.75 |
| ATOM | 3072 | CG1 | ILE B 104 | 48.085 | 22.913 | 61.452 | 1.000 | 27.91 |
| ATOM | 3073 | CD1 | ILE B 104 | 48.886 | 21.643 | 61.328 | 1.000 | 18.81 |
| ATOM | 3074 | CG2 | ILE B 104 | 46.164 | 21.938 | 60.144 | 1.000 | 20.62 |
| ATOM | 3075 | C   | ILE B 104 | 46.672 | 23.774 | 57.966 | 1.000 | 24.01 |
| ATOM | 3076 | O   | ILE B 104 | 46.080 | 24.847 | 58.018 | 1.000 | 15.86 |
| ATOM | 3077 | N   | PRO B 105 | 46.370 | 22.829 | 57.086 | 1.000 | 25.98 |
| ATOM | 3078 | CA  | PRO B 105 | 45.332 | 23.074 | 56.078 | 1.000 | 27.95 |
| ATOM | 3079 | CB  | PRO B 105 | 45.503 | 21.922 | 55.088 | 1.000 | 18.03 |
| ATOM | 3080 | CG  | PRO B 105 | 46.582 | 21.035 | 55.586 | 1.000 | 21.67 |
| ATOM | 3081 | CD  | PRO B 105 | 46.944 | 21.482 | 56.973 | 1.000 | 24.89 |
| ATOM | 3082 | C   | PRO B 105 | 43.940 | 23.045 | 56.698 | 1.000 | 28.32 |
| ATOM | 3083 | O   | PRO B 105 | 43.656 | 22.391 | 57.703 | 1.000 | 36.85 |
| ATOM | 3084 | N   | GLY B 106 | 43.011 | 23.768 | 56.085 | 1.000 | 21.37 |
| ATOM | 3085 | CA  | GLY B 106 | 41.640 | 23.703 | 56.591 | 1.000 | 21.21 |
| ATOM | 3086 | C   | GLY B 106 | 40.757 | 23.172 | 55.465 | 1.000 | 27.66 |
| ATOM | 3087 | O   | GLY B 106 | 41.280 | 22.580 | 54.521 | 1.000 | 21.69 |
| ATOM | 3088 | N   | ASN B 107 | 39.461 | 23.394 | 55.567 | 1.000 | 27.43 |
| ATOM | 3089 | CA  | ASN B 107 | 38.490 | 22.979 | 54.572 | 1.000 | 35.96 |
| ATOM | 3090 | CB  | ASN B 107 | 37.085 | 23.184 | 55.152 | 1.000 | 47.76 |
| ATOM | 3091 | CG  | ASN B 107 | 36.304 | 21.899 | 55.308 | 1.000 | 49.77 |
| ATOM | 3092 | OD1 | ASN B 107 | 35.075 | 21.945 | 55.229 | 1.000 | 73.31 |
| ATOM | 3093 | ND2 | ASN B 107 | 36.983 | 20.777 | 55.521 | 1.000 | 41.72 |
| ATOM | 3094 | C   | ASN B 107 | 38.605 | 23.762 | 53.268 | 1.000 | 40.01 |
| ATOM | 3095 | O   | ASN B 107 | 38.170 | 23.268 | 52.227 | 1.000 | 27.43 |
| ATOM | 3096 | N   | ASN B 108 | 39.172 | 24.962 | 53.316 | 1.000 | 47.34 |
| ATOM | 3097 | CA  | ASN B 108 | 39.181 | 25.892 | 52.194 | 1.000 | 49.18 |
| ATOM | 3098 | CB  | ASN B 108 | 38.573 | 27.227 | 52.670 | 1.000 | 53.17 |
| ATOM | 3099 | CG  | ASN B 108 | 37.444 | 27.012 | 53.664 | 1.000 | 60.31 |
| ATOM | 3100 | OD1 | ASN B 108 | 36.332 | 26.632 | 53.279 | 1.000 | 45.80 |
| ATOM | 3101 | ND2 | ASN B 108 | 37.724 | 27.248 | 54.945 | 1.000 | 39.45 |
| ATOM | 3102 | C   | ASN B 108 | 40.545 | 26.159 | 51.574 | 1.000 | 41.89 |
| ATOM | 3103 | O   | ASN B 108 | 40.633 | 26.284 | 50.347 | 1.000 | 48.34 |
| ATOM | 3104 | N   | PHE B 109 | 41.607 | 26.266 | 52.373 | 1.000 | 32.76 |
| ATOM | 3105 | CA  | PHE B 109 | 42.947 | 26.513 | 51.844 | 1.000 | 22.32 |
| ATOM | 3106 | CB  | PHE B 109 | 43.245 | 28.009 | 51.738 | 1.000 | 27.58 |
| ATOM | 3107 | CG  | PHE B 109 | 42.837 | 28.902 | 52.878 | 1.000 | 36.26 |
| ATOM | 3108 | CD1 | PHE B 109 | 43.785 | 29.482 | 53.709 | 1.000 | 36.93 |
| ATOM | 3109 | CE1 | PHE B 109 | 43.434 | 30.318 | 54.748 | 1.000 | 43.65 |
| ATOM | 3110 | CZ  | PHE B 109 | 42.102 | 30.599 | 54.991 | 1.000 | 46.87 |
| ATOM | 3111 | CE2 | PHE B 109 | 41.144 | 30.029 | 54.175 | 1.000 | 48.29 |
| ATOM | 3112 | CD2 | PHE B 109 | 41.509 | 29.191 | 53.140 | 1.000 | 38.59 |
| ATOM | 3113 | C   | PHE B 109 | 44.009 | 25.809 | 52.681 | 1.000 | 26.82 |
| ATOM | 3114 | O   | PHE B 109 | 43.745 | 25.302 | 53.775 | 1.000 | 33.42 |
| ATOM | 3115 | N   | ARG B 110 | 45.231 | 25.760 | 52.163 | 1.000 | 21.41 |
| ATOM | 3116 | CA  | ARG B 110 | 46.293 | 24.976 | 52.783 | 1.000 | 29.86 |
| ATOM | 3117 | CB  | ARG B 110 | 47.331 | 24.635 | 51.691 | 1.000 | 23.08 |
| ATOM | 3118 | CG  | ARG B 110 | 46.678 | 23.836 | 50.567 | 1.000 | 24.73 |
| ATOM | 3119 | CD  | ARG B 110 | 47.700 | 23.142 | 49.690 | 1.000 | 35.94 |

**FIGURE 66**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3120 | NE  | ARG | B | 110 | 48.602 | 22.284 | 50.447 | 1.000 | 54.44 |
| ATOM | 3121 | CZ  | ARG | B | 110 | 48.689 | 20.963 | 50.337 | 1.000 | 65.83 |
| ATOM | 3122 | NH1 | ARG | B | 110 | 47.907 | 20.318 | 49.480 | 1.000 | 62.56 |
| ATOM | 3123 | NH2 | ARG | B | 110 | 49.562 | 20.304 | 51.095 | 1.000 | 60.21 |
| ATOM | 3124 | C   | ARG | B | 110 | 46.975 | 25.640 | 53.960 | 1.000 | 33.08 |
| ATOM | 3125 | O   | ARG | B | 110 | 47.566 | 24.963 | 54.817 | 1.000 | 25.95 |
| ATOM | 3126 | N   | ARG | B | 111 | 46.949 | 26.968 | 54.073 | 1.000 | 29.38 |
| ATOM | 3127 | CA  | ARG | B | 111 | 47.600 | 27.571 | 55.248 | 1.000 | 25.02 |
| ATOM | 3128 | CB  | ARG | B | 111 | 48.716 | 28.513 | 54.839 | 1.000 | 22.60 |
| ATOM | 3129 | CG  | ARG | B | 111 | 49.940 | 27.889 | 54.187 | 1.000 | 25.96 |
| ATOM | 3130 | CD  | ARG | B | 111 | 51.044 | 28.951 | 54.077 | 1.000 | 25.11 |
| ATOM | 3131 | NE  | ARG | B | 111 | 52.352 | 28.321 | 54.010 | 1.000 | 31.63 |
| ATOM | 3132 | CZ  | ARG | B | 111 | 53.527 | 28.919 | 53.942 | 1.000 | 26.99 |
| ATOM | 3133 | NH1 | ARG | B | 111 | 53.614 | 30.238 | 53.935 | 1.000 | 28.95 |
| ATOM | 3134 | NH2 | ARG | B | 111 | 54.622 | 28.173 | 53.884 | 1.000 | 31.47 |
| ATOM | 3135 | C   | ARG | B | 111 | 46.556 | 28.306 | 56.085 | 1.000 | 24.94 |
| ATOM | 3136 | O   | ARG | B | 111 | 46.687 | 29.475 | 56.447 | 1.000 | 29.91 |
| ATOM | 3137 | N   | GLU | B | 112 | 45.493 | 27.571 | 56.391 | 1.000 | 23.64 |
| ATOM | 3138 | CA  | GLU | B | 112 | 44.323 | 28.134 | 57.049 | 1.000 | 17.42 |
| ATOM | 3139 | CB  | GLU | B | 112 | 43.130 | 27.204 | 56.817 | 1.000 | 18.28 |
| ATOM | 3140 | CG  | GLU | B | 112 | 41.790 | 27.862 | 57.105 | 1.000 | 24.48 |
| ATOM | 3141 | CD  | GLU | B | 112 | 40.654 | 27.199 | 56.351 | 1.000 | 26.29 |
| ATOM | 3142 | OE1 | GLU | B | 112 | 39.501 | 27.461 | 56.751 | 1.000 | 26.21 |
| ATOM | 3143 | OE2 | GLU | B | 112 | 40.909 | 26.434 | 55.398 | 1.000 | 31.20 |
| ATOM | 3144 | C   | GLU | B | 112 | 44.592 | 28.379 | 58.528 | 1.000 | 17.73 |
| ATOM | 3145 | O   | GLU | B | 112 | 44.083 | 29.339 | 59.110 | 1.000 | 22.88 |
| ATOM | 3146 | N   | TYR | B | 113 | 45.416 | 27.518 | 59.101 | 1.000 | 16.08 |
| ATOM | 3147 | CA  | TYR | B | 113 | 45.780 | 27.574 | 60.502 | 1.000 | 21.42 |
| ATOM | 3148 | CB  | TYR | B | 113 | 45.177 | 26.393 | 61.277 | 1.000 | 23.13 |
| ATOM | 3149 | CG  | TYR | B | 113 | 43.707 | 26.143 | 61.023 | 1.000 | 21.61 |
| ATOM | 3150 | CD1 | TYR | B | 113 | 43.282 | 25.255 | 60.046 | 1.000 | 20.99 |
| ATOM | 3151 | CE1 | TYR | B | 113 | 41.933 | 25.027 | 59.815 | 1.000 | 20.86 |
| ATOM | 3152 | CZ  | TYR | B | 113 | 40.987 | 25.692 | 60.567 | 1.000 | 21.97 |
| ATOM | 3153 | OH  | TYR | B | 113 | 39.644 | 25.476 | 60.352 | 1.000 | 20.75 |
| ATOM | 3154 | CE2 | TYR | B | 113 | 41.385 | 26.582 | 61.546 | 1.000 | 21.97 |
| ATOM | 3155 | CD2 | TYR | B | 113 | 42.735 | 26.804 | 61.770 | 1.000 | 21.68 |
| ATOM | 3156 | C   | TYR | B | 113 | 47.295 | 27.552 | 60.685 | 1.000 | 27.43 |
| ATOM | 3157 | O   | TYR | B | 113 | 48.024 | 26.950 | 59.899 | 1.000 | 18.10 |
| ATOM | 3158 | N   | ILE | B | 114 | 47.733 | 28.214 | 61.752 | 1.000 | 19.17 |
| ATOM | 3159 | CA  | ILE | B | 114 | 49.024 | 27.953 | 62.338 | 1.000 | 17.32 |
| ATOM | 3160 | CB  | ILE | B | 114 | 49.919 | 29.192 | 62.464 | 1.000 | 22.32 |
| ATOM | 3161 | CG1 | ILE | B | 114 | 50.399 | 29.756 | 61.124 | 1.000 | 15.29 |
| ATOM | 3162 | CD1 | ILE | B | 114 | 50.784 | 31.212 | 61.142 | 1.000 | 18.68 |
| ATOM | 3163 | CG2 | ILE | B | 114 | 51.079 | 28.849 | 63.390 | 1.000 | 21.25 |
| ATOM | 3164 | C   | ILE | B | 114 | 48.786 | 27.336 | 63.725 | 1.000 | 21.28 |
| ATOM | 3165 | O   | ILE | B | 114 | 48.140 | 27.927 | 64.594 | 1.000 | 17.78 |
| ATOM | 3166 | N   | VAL | B | 115 | 49.305 | 26.125 | 63.911 | 1.000 | 17.69 |
| ATOM | 3167 | CA  | VAL | B | 115 | 49.196 | 25.470 | 65.217 | 1.000 | 24.09 |
| ATOM | 3168 | CB  | VAL | B | 115 | 48.867 | 23.969 | 65.081 | 1.000 | 25.84 |
| ATOM | 3169 | CG1 | VAL | B | 115 | 49.290 | 23.223 | 66.338 | 1.000 | 28.88 |
| ATOM | 3170 | CG2 | VAL | B | 115 | 47.385 | 23.774 | 64.788 | 1.000 | 23.07 |
| ATOM | 3171 | C   | VAL | B | 115 | 50.500 | 25.641 | 65.985 | 1.000 | 22.51 |

**FIGURE 67**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3172 | O   | VAL | B | 115 | 51.594 | 25.418 | 65.450 | 1.000 | 14.78 |
| ATOM | 3173 | N   | THR | B | 116 | 50.429 | 26.049 | 67.251 | 1.000 | 21.02 |
| ATOM | 3174 | CA  | THR | B | 116 | 51.704 | 26.242 | 67.962 | 1.000 | 19.77 |
| ATOM | 3175 | CB  | THR | B | 116 | 52.149 | 27.711 | 67.869 | 1.000 | 23.82 |
| ATOM | 3176 | OG1 | THR | B | 116 | 53.495 | 27.907 | 68.350 | 1.000 | 16.84 |
| ATOM | 3177 | CG2 | THR | B | 116 | 51.242 | 28.587 | 68.722 | 1.000 | 19.85 |
| ATOM | 3178 | C   | THR | B | 116 | 51.552 | 25.744 | 69.390 | 1.000 | 22.67 |
| ATOM | 3179 | O   | THR | B | 116 | 50.467 | 25.376 | 69.849 | 1.000 | 17.14 |
| ATOM | 3180 | N   | GLN | B | 117 | 52.654 | 25.693 | 70.119 | 1.000 | 23.60 |
| ATOM | 3181 | CA  | GLN | B | 117 | 52.679 | 25.319 | 71.514 | 1.000 | 23.36 |
| ATOM | 3182 | CB  | GLN | B | 117 | 54.080 | 24.807 | 71.898 | 1.000 | 24.62 |
| ATOM | 3183 | CG  | GLN | B | 117 | 55.034 | 25.933 | 72.239 | 1.000 | 18.72 |
| ATOM | 3184 | CD  | GLN | B | 117 | 56.479 | 25.515 | 72.375 | 1.000 | 26.17 |
| ATOM | 3185 | OE1 | GLN | B | 117 | 56.812 | 24.331 | 72.431 | 1.000 | 27.92 |
| ATOM | 3186 | NE2 | GLN | B | 117 | 57.357 | 26.520 | 72.419 | 1.000 | 23.64 |
| ATOM | 3187 | C   | GLN | B | 117 | 52.327 | 26.512 | 72.391 | 1.000 | 23.75 |
| ATOM | 3188 | O   | GLN | B | 117 | 52.440 | 27.656 | 71.939 | 1.000 | 18.82 |
| ATOM | 3189 | N   | GLY | B | 118 | 51.927 | 26.261 | 73.638 | 1.000 | 21.15 |
| ATOM | 3190 | CA  | GLY | B | 118 | 51.716 | 27.416 | 74.523 | 1.000 | 21.52 |
| ATOM | 3191 | C   | GLY | B | 118 | 53.050 | 28.104 | 74.761 | 1.000 | 17.96 |
| ATOM | 3192 | O   | GLY | B | 118 | 54.002 | 27.456 | 75.207 | 1.000 | 23.95 |
| ATOM | 3193 | N   | PRO | B | 119 | 53.131 | 29.390 | 74.454 | 1.000 | 18.88 |
| ATOM | 3194 | CA  | PRO | B | 119 | 54.401 | 30.117 | 74.548 | 1.000 | 23.38 |
| ATOM | 3195 | CB  | PRO | B | 119 | 53.993 | 31.581 | 74.327 | 1.000 | 19.87 |
| ATOM | 3196 | CG  | PRO | B | 119 | 52.757 | 31.486 | 73.500 | 1.000 | 19.60 |
| ATOM | 3197 | CD  | PRO | B | 119 | 52.031 | 30.260 | 74.000 | 1.000 | 17.07 |
| ATOM | 3198 | C   | PRO | B | 119 | 55.064 | 29.980 | 75.917 | 1.000 | 25.74 |
| ATOM | 3199 | O   | PRO | B | 119 | 54.414 | 29.867 | 76.952 | 1.000 | 21.95 |
| ATOM | 3200 | N   | LEU | B | 120 | 56.384 | 29.996 | 75.884 | 1.000 | 24.68 |
| ATOM | 3201 | CA  | LEU | B | 120 | 57.259 | 29.997 | 77.034 | 1.000 | 28.37 |
| ATOM | 3202 | CB  | LEU | B | 120 | 58.542 | 29.210 | 76.755 | 1.000 | 21.91 |
| ATOM | 3203 | CG  | LEU | B | 120 | 58.366 | 27.711 | 76.511 | 1.000 | 23.23 |
| ATOM | 3204 | CD1 | LEU | B | 120 | 59.490 | 27.175 | 75.642 | 1.000 | 25.39 |
| ATOM | 3205 | CD2 | LEU | B | 120 | 58.314 | 26.965 | 77.837 | 1.000 | 31.44 |
| ATOM | 3206 | C   | LEU | B | 120 | 57.615 | 31.439 | 77.377 | 1.000 | 22.77 |
| ATOM | 3207 | O   | LEU | B | 120 | 57.514 | 32.304 | 76.499 | 1.000 | 23.03 |
| ATOM | 3208 | N   | PRO | B | 121 | 58.016 | 31.692 | 78.615 | 1.000 | 26.35 |
| ATOM | 3209 | CA  | PRO | B | 121 | 58.561 | 33.014 | 78.945 | 1.000 | 22.57 |
| ATOM | 3210 | CB  | PRO | B | 121 | 59.171 | 32.787 | 80.326 | 1.000 | 27.81 |
| ATOM | 3211 | CG  | PRO | B | 121 | 58.375 | 31.675 | 80.918 | 1.000 | 32.45 |
| ATOM | 3212 | CD  | PRO | B | 121 | 57.975 | 30.783 | 79.773 | 1.000 | 28.73 |
| ATOM | 3213 | C   | PRO | B | 121 | 59.641 | 33.414 | 77.943 | 1.000 | 28.24 |
| ATOM | 3214 | O   | PRO | B | 121 | 59.741 | 34.555 | 77.489 | 1.000 | 30.29 |
| ATOM | 3215 | N   | GLY | B | 122 | 60.489 | 32.450 | 77.562 | 1.000 | 22.78 |
| ATOM | 3216 | CA  | GLY | B | 122 | 61.573 | 32.788 | 76.653 | 1.000 | 20.37 |
| ATOM | 3217 | C   | GLY | B | 122 | 61.178 | 32.799 | 75.191 | 1.000 | 28.02 |
| ATOM | 3218 | O   | GLY | B | 122 | 61.990 | 33.229 | 74.365 | 1.000 | 28.41 |
| ATOM | 3219 | N   | THR | B | 123 | 59.980 | 32.360 | 74.810 | 1.000 | 27.99 |
| ATOM | 3220 | CA  | THR | B | 123 | 59.604 | 32.385 | 73.401 | 1.000 | 33.24 |
| ATOM | 3221 | CB  | THR | B | 123 | 59.259 | 30.981 | 72.854 | 1.000 | 33.57 |
| ATOM | 3222 | OG1 | THR | B | 123 | 58.039 | 30.554 | 73.480 | 1.000 | 25.65 |
| ATOM | 3223 | CG2 | THR | B | 123 | 60.341 | 29.968 | 73.169 | 1.000 | 20.05 |

FIGURE 68



|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3224 | C   | THR | B | 123 | 58.385 | 33.260 | 73.106 | 1.000 | 29.44 |
| ATOM | 3225 | O   | THR | B | 123 | 57.931 | 33.303 | 71.961 | 1.000 | 25.91 |
| ATOM | 3226 | N   | LYS | B | 124 | 57.853 | 33.950 | 74.105 | 1.000 | 26.51 |
| ATOM | 3227 | CA  | LYS | B | 124 | 56.691 | 34.807 | 73.893 | 1.000 | 28.23 |
| ATOM | 3228 | CB  | LYS | B | 124 | 56.273 | 35.483 | 75.199 | 1.000 | 32.16 |
| ATOM | 3229 | CG  | LYS | B | 124 | 57.460 | 35.814 | 76.097 | 1.000 | 43.91 |
| ATOM | 3230 | CD  | LYS | B | 124 | 57.144 | 37.009 | 76.981 | 1.000 | 56.45 |
| ATOM | 3231 | CE  | LYS | B | 124 | 57.277 | 36.684 | 78.458 | 1.000 | 47.68 |
| ATOM | 3232 | NZ  | LYS | B | 124 | 56.082 | 37.130 | 79.224 | 1.000 | 47.04 |
| ATOM | 3233 | C   | LYS | B | 124 | 56.961 | 35.882 | 72.845 | 1.000 | 31.27 |
| ATOM | 3234 | O   | LYS | B | 124 | 56.010 | 36.336 | 72.203 | 1.000 | 20.04 |
| ATOM | 3235 | N   | ASP | B | 125 | 58.221 | 36.273 | 72.690 | 1.000 | 27.24 |
| ATOM | 3236 | CA  | ASP | B | 125 | 58.589 | 37.344 | 71.759 | 1.000 | 30.97 |
| ATOM | 3237 | CB  | ASP | B | 125 | 59.998 | 37.856 | 72.044 | 1.000 | 30.13 |
| ATOM | 3238 | CG  | ASP | B | 125 | 60.063 | 38.882 | 73.163 | 1.000 | 37.62 |
| ATOM | 3239 | OD1 | ASP | B | 125 | 59.010 | 39.337 | 73.647 | 1.000 | 29.79 |
| ATOM | 3240 | OD2 | ASP | B | 125 | 61.180 | 39.261 | 73.577 | 1.000 | 55.37 |
| ATOM | 3241 | C   | ASP | B | 125 | 58.486 | 36.861 | 70.313 | 1.000 | 29.10 |
| ATOM | 3242 | O   | ASP | B | 125 | 58.053 | 37.590 | 69.423 | 1.000 | 23.13 |
| ATOM | 3243 | N   | ASP | B | 126 | 58.894 | 35.619 | 70.119 | 1.000 | 29.81 |
| ATOM | 3244 | CA  | ASP | B | 126 | 58.855 | 34.917 | 68.846 | 1.000 | 29.93 |
| ATOM | 3245 | CB  | ASP | B | 126 | 59.612 | 33.590 | 68.923 | 1.000 | 33.34 |
| ATOM | 3246 | CG  | ASP | B | 126 | 61.095 | 33.725 | 69.208 | 1.000 | 42.49 |
| ATOM | 3247 | OD1 | ASP | B | 126 | 61.684 | 34.754 | 68.799 | 1.000 | 33.29 |
| ATOM | 3248 | OD2 | ASP | B | 126 | 61.666 | 32.798 | 69.837 | 1.000 | 36.63 |
| ATOM | 3249 | C   | ASP | B | 126 | 57.410 | 34.663 | 68.425 | 1.000 | 29.50 |
| ATOM | 3250 | O   | ASP | B | 126 | 57.077 | 34.759 | 67.243 | 1.000 | 23.31 |
| ATOM | 3251 | N   | PHE | B | 127 | 56.556 | 34.333 | 69.391 | 1.000 | 27.35 |
| ATOM | 3252 | CA  | PHE | B | 127 | 55.135 | 34.135 | 69.089 | 1.000 | 28.78 |
| ATOM | 3253 | CB  | PHE | B | 127 | 54.360 | 33.783 | 70.363 | 1.000 | 25.58 |
| ATOM | 3254 | CG  | PHE | B | 127 | 52.860 | 33.698 | 70.240 | 1.000 | 22.20 |
| ATOM | 3255 | CD1 | PHE | B | 127 | 52.255 | 32.500 | 69.878 | 1.000 | 21.35 |
| ATOM | 3256 | CE1 | PHE | B | 127 | 50.881 | 32.398 | 69.750 | 1.000 | 20.50 |
| ATOM | 3257 | CZ  | PHE | B | 127 | 50.087 | 33.500 | 70.006 | 1.000 | 26.34 |
| ATOM | 3258 | CE2 | PHE | B | 127 | 50.667 | 34.705 | 70.361 | 1.000 | 17.31 |
| ATOM | 3259 | CD2 | PHE | B | 127 | 52.039 | 34.789 | 70.487 | 1.000 | 15.23 |
| ATOM | 3260 | C   | PHE | B | 127 | 54.535 | 35.373 | 68.426 | 1.000 | 22.38 |
| ATOM | 3261 | O   | PHE | B | 127 | 53.905 | 35.276 | 67.377 | 1.000 | 24.96 |
| ATOM | 3262 | N   | TRP | B | 128 | 54.685 | 36.549 | 69.032 | 1.000 | 24.70 |
| ATOM | 3263 | CA  | TRP | B | 128 | 54.065 | 37.773 | 68.523 | 1.000 | 19.09 |
| ATOM | 3264 | CB  | TRP | B | 128 | 54.104 | 38.859 | 69.604 | 1.000 | 17.25 |
| ATOM | 3265 | CG  | TRP | B | 128 | 53.145 | 38.614 | 70.734 | 1.000 | 17.80 |
| ATOM | 3266 | CD1 | TRP | B | 128 | 53.470 | 38.390 | 72.040 | 1.000 | 22.53 |
| ATOM | 3267 | NE1 | TRP | B | 128 | 52.331 | 38.203 | 72.789 | 1.000 | 21.74 |
| ATOM | 3268 | CE2 | TRP | B | 128 | 51.240 | 38.303 | 71.966 | 1.000 | 19.23 |
| ATOM | 3269 | CD2 | TRP | B | 128 | 51.714 | 38.558 | 70.668 | 1.000 | 19.24 |
| ATOM | 3270 | CE3 | TRP | B | 128 | 50.778 | 38.703 | 69.637 | 1.000 | 28.93 |
| ATOM | 3271 | CZ3 | TRP | B | 128 | 49.429 | 38.592 | 69.915 | 1.000 | 22.05 |
| ATOM | 3272 | CH2 | TRP | B | 128 | 48.991 | 38.335 | 71.226 | 1.000 | 17.91 |
| ATOM | 3273 | CZ2 | TRP | B | 128 | 49.878 | 38.187 | 72.259 | 1.000 | 22.46 |
| ATOM | 3274 | C   | TRP | B | 128 | 54.735 | 38.234 | 67.237 | 1.000 | 18.56 |
| ATOM | 3275 | O   | TRP | B | 128 | 54.116 | 38.775 | 66.322 | 1.000 | 21.01 |

**FIGURE 69**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3276 | N   | LYS | B | 129 | 56.042 | 38.016 | 67.133 | 1.000 | 13.97 |
| ATOM | 3277 | CA  | LYS | B | 129 | 56.723 | 38.282 | 65.866 | 1.000 | 15.64 |
| ATOM | 3278 | CB  | LYS | B | 129 | 58.217 | 37.994 | 65.979 | 1.000 | 22.55 |
| ATOM | 3279 | CG  | LYS | B | 129 | 58.950 | 37.985 | 64.651 | 1.000 | 39.82 |
| ATOM | 3280 | CD  | LYS | B | 129 | 60.460 | 38.047 | 64.814 | 1.000 | 48.10 |
| ATOM | 3281 | CE  | LYS | B | 129 | 61.160 | 37.738 | 63.491 | 1.000 | 52.05 |
| ATOM | 3282 | NZ  | LYS | B | 129 | 62.627 | 37.573 | 63.678 | 1.000 | 61.20 |
| ATOM | 3283 | C   | LYS | B | 129 | 56.113 | 37.409 | 64.776 | 1.000 | 27.27 |
| ATOM | 3284 | O   | LYS | B | 129 | 55.893 | 37.876 | 63.661 | 1.000 | 29.01 |
| ATOM | 3285 | N   | MET | B | 130 | 55.848 | 36.148 | 65.124 | 1.000 | 29.80 |
| ATOM | 3286 | CA  | MET | B | 130 | 55.154 | 35.233 | 64.230 | 1.000 | 27.17 |
| ATOM | 3287 | CB  | MET | B | 130 | 54.979 | 33.827 | 64.845 | 1.000 | 19.02 |
| ATOM | 3288 | CG  | MET | B | 130 | 54.169 | 32.925 | 63.904 | 1.000 | 19.86 |
| ATOM | 3289 | SD  | MET | B | 130 | 54.092 | 31.205 | 64.479 | 1.000 | 25.65 |
| ATOM | 3290 | CE  | MET | B | 130 | 52.919 | 31.427 | 65.833 | 1.000 | 14.58 |
| ATOM | 3291 | C   | MET | B | 130 | 53.777 | 35.775 | 63.863 | 1.000 | 17.87 |
| ATOM | 3292 | O   | MET | B | 130 | 53.351 | 35.838 | 62.715 | 1.000 | 21.77 |
| ATOM | 3293 | N   | VAL | B | 131 | 53.029 | 36.170 | 64.886 | 1.000 | 12.63 |
| ATOM | 3294 | CA  | VAL | B | 131 | 51.706 | 36.739 | 64.639 | 1.000 | 19.47 |
| ATOM | 3295 | CB  | VAL | B | 131 | 51.028 | 37.081 | 65.977 | 1.000 | 24.44 |
| ATOM | 3296 | CG1 | VAL | B | 131 | 49.870 | 38.035 | 65.754 | 1.000 | 20.24 |
| ATOM | 3297 | CG2 | VAL | B | 131 | 50.586 | 35.801 | 66.687 | 1.000 | 20.58 |
| ATOM | 3298 | C   | VAL | B | 131 | 51.794 | 37.977 | 63.748 | 1.000 | 29.32 |
| ATOM | 3299 | O   | VAL | B | 131 | 50.974 | 38.203 | 62.851 | 1.000 | 27.58 |
| ATOM | 3300 | N   | TRP | B | 132 | 52.810 | 38.804 | 63.985 | 1.000 | 24.33 |
| ATOM | 3301 | CA  | TRP | B | 132 | 52.980 | 40.015 | 63.177 | 1.000 | 25.60 |
| ATOM | 3302 | CB  | TRP | B | 132 | 54.037 | 40.918 | 63.807 | 1.000 | 21.12 |
| ATOM | 3303 | CG  | TRP | B | 132 | 54.280 | 42.211 | 63.101 | 1.000 | 30.16 |
| ATOM | 3304 | CD1 | TRP | B | 132 | 55.382 | 42.547 | 62.364 | 1.000 | 34.45 |
| ATOM | 3305 | NE1 | TRP | B | 132 | 55.258 | 43.822 | 61.863 | 1.000 | 35.96 |
| ATOM | 3306 | CE2 | TRP | B | 132 | 54.059 | 44.338 | 62.273 | 1.000 | 34.79 |
| ATOM | 3307 | CD2 | TRP | B | 132 | 53.417 | 43.354 | 63.054 | 1.000 | 29.88 |
| ATOM | 3308 | CE3 | TRP | B | 132 | 52.159 | 43.629 | 63.598 | 1.000 | 23.47 |
| ATOM | 3309 | CZ3 | TRP | B | 132 | 51.604 | 44.866 | 63.343 | 1.000 | 29.19 |
| ATOM | 3310 | CH2 | TRP | B | 132 | 52.271 | 45.821 | 62.564 | 1.000 | 30.89 |
| ATOM | 3311 | CZ2 | TRP | B | 132 | 53.499 | 45.590 | 62.016 | 1.000 | 31.90 |
| ATOM | 3312 | C   | TRP | B | 132 | 53.348 | 39.679 | 61.736 | 1.000 | 27.64 |
| ATOM | 3313 | O   | TRP | B | 132 | 52.732 | 40.210 | 60.809 | 1.000 | 25.13 |
| ATOM | 3314 | N   | GLU | B | 133 | 54.336 | 38.817 | 61.516 | 1.000 | 19.97 |
| ATOM | 3315 | CA  | GLU | B | 133 | 54.803 | 38.528 | 60.167 | 1.000 | 21.72 |
| ATOM | 3316 | CB  | GLU | B | 133 | 56.122 | 37.762 | 60.268 | 1.000 | 25.50 |
| ATOM | 3317 | CG  | GLU | B | 133 | 57.215 | 38.565 | 60.953 | 1.000 | 21.80 |
| ATOM | 3318 | CD  | GLU | B | 133 | 58.525 | 37.797 | 60.960 | 1.000 | 30.30 |
| ATOM | 3319 | OE1 | GLU | B | 133 | 58.479 | 36.560 | 60.767 | 1.000 | 25.13 |
| ATOM | 3320 | OE2 | GLU | B | 133 | 59.568 | 38.461 | 61.151 | 1.000 | 35.58 |
| ATOM | 3321 | C   | GLU | B | 133 | 53.810 | 37.732 | 59.339 | 1.000 | 28.77 |
| ATOM | 3322 | O   | GLU | B | 133 | 53.729 | 37.935 | 58.127 | 1.000 | 26.53 |
| ATOM | 3323 | N   | GLN | B | 134 | 53.050 | 36.828 | 59.957 | 1.000 | 25.47 |
| ATOM | 3324 | CA  | GLN | B | 134 | 52.103 | 36.010 | 59.204 | 1.000 | 24.21 |
| ATOM | 3325 | CB  | GLN | B | 134 | 51.962 | 34.639 | 59.875 | 1.000 | 30.73 |
| ATOM | 3326 | CG  | GLN | B | 134 | 53.313 | 33.951 | 60.093 | 1.000 | 29.62 |
| ATOM | 3327 | CD  | GLN | B | 134 | 53.852 | 33.400 | 58.783 | 1.000 | 30.05 |

**FIGURE 70**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3328 | OE1 | GLN | B | 134 | 53.182 | 32.656 | 58.068 | 1.000 | 33.53 |
| ATOM | 3329 | NE2 | GLN | B | 134 | 55.080 | 33.772 | 58.460 | 1.000 | 33.18 |
| ATOM | 3330 | C   | GLN | B | 134 | 50.739 | 36.668 | 59.092 | 1.000 | 26.45 |
| ATOM | 3331 | O   | GLN | B | 134 | 49.769 | 36.050 | 58.640 | 1.000 | 25.94 |
| ATOM | 3332 | N   | ASN | B | 135 | 50.646 | 37.924 | 59.510 | 1.000 | 24.63 |
| ATOM | 3333 | CA  | ASN | B | 135 | 49.405 | 38.687 | 59.374 | 1.000 | 25.47 |
| ATOM | 3334 | CB  | ASN | B | 135 | 49.089 | 38.902 | 57.885 | 1.000 | 27.21 |
| ATOM | 3335 | CG  | ASN | B | 135 | 49.300 | 40.369 | 57.529 | 1.000 | 46.77 |
| ATOM | 3336 | OD1 | ASN | B | 135 | 48.353 | 41.121 | 57.307 | 1.000 | 69.94 |
| ATOM | 3337 | ND2 | ASN | B | 135 | 50.565 | 40.770 | 57.500 | 1.000 | 36.37 |
| ATOM | 3338 | C   | ASN | B | 135 | 48.223 | 38.027 | 60.069 | 1.000 | 31.62 |
| ATOM | 3339 | O   | ASN | B | 135 | 47.088 | 38.019 | 59.589 | 1.000 | 28.84 |
| ATOM | 3340 | N   | VAL | B | 136 | 48.484 | 37.467 | 61.246 | 1.000 | 27.43 |
| ATOM | 3341 | CA  | VAL | B | 136 | 47.416 | 36.859 | 62.032 | 1.000 | 24.98 |
| ATOM | 3342 | CB  | VAL | B | 136 | 48.035 | 36.029 | 63.179 | 1.000 | 20.72 |
| ATOM | 3343 | CG1 | VAL | B | 136 | 46.958 | 35.491 | 64.102 | 1.000 | 26.47 |
| ATOM | 3344 | CG2 | VAL | B | 136 | 48.887 | 34.909 | 62.599 | 1.000 | 13.70 |
| ATOM | 3345 | C   | VAL | B | 136 | 46.469 | 37.891 | 62.619 | 1.000 | 23.98 |
| ATOM | 3346 | O   | VAL | B | 136 | 46.875 | 38.904 | 63.196 | 1.000 | 19.31 |
| ATOM | 3347 | N   | HIS | B | 137 | 45.165 | 37.662 | 62.502 | 1.000 | 24.96 |
| ATOM | 3348 | CA  | HIS | B | 137 | 44.208 | 38.529 | 63.180 | 1.000 | 24.73 |
| ATOM | 3349 | CB  | HIS | B | 137 | 43.215 | 39.124 | 62.170 | 1.000 | 30.08 |
| ATOM | 3350 | CG  | HIS | B | 137 | 43.872 | 40.090 | 61.240 | 1.000 | 35.97 |
| ATOM | 3351 | ND1 | HIS | B | 137 | 43.604 | 41.435 | 61.247 | 1.000 | 47.37 |
| ATOM | 3352 | CE1 | HIS | B | 137 | 44.338 | 42.022 | 60.314 | 1.000 | 50.81 |
| ATOM | 3353 | NE2 | HIS | B | 137 | 45.073 | 41.107 | 59.706 | 1.000 | 44.95 |
| ATOM | 3354 | CD2 | HIS | B | 137 | 44.799 | 39.891 | 60.275 | 1.000 | 40.02 |
| ATOM | 3355 | C   | HIS | B | 137 | 43.407 | 37.801 | 64.253 | 1.000 | 21.29 |
| ATOM | 3356 | O   | HIS | B | 137 | 42.727 | 38.467 | 65.026 | 1.000 | 27.23 |
| ATOM | 3357 | N   | ASN | B | 138 | 43.469 | 36.470 | 64.274 | 1.000 | 22.17 |
| ATOM | 3358 | CA  | ASN | B | 138 | 42.685 | 35.702 | 65.233 | 1.000 | 20.26 |
| ATOM | 3359 | CB  | ASN | B | 138 | 41.491 | 35.030 | 64.534 | 1.000 | 26.81 |
| ATOM | 3360 | CG  | ASN | B | 138 | 40.525 | 36.056 | 63.968 | 1.000 | 33.07 |
| ATOM | 3361 | OD1 | ASN | B | 138 | 40.383 | 36.164 | 62.750 | 1.000 | 31.33 |
| ATOM | 3362 | ND2 | ASN | B | 138 | 39.869 | 36.819 | 64.842 | 1.000 | 20.76 |
| ATOM | 3363 | C   | ASN | B | 138 | 43.540 | 34.655 | 65.938 | 1.000 | 23.24 |
| ATOM | 3364 | O   | ASN | B | 138 | 44.238 | 33.895 | 65.262 | 1.000 | 18.61 |
| ATOM | 3365 | N   | ILE | B | 139 | 43.462 | 34.638 | 67.266 | 1.000 | 19.79 |
| ATOM | 3366 | CA  | ILE | B | 139 | 44.122 | 33.625 | 68.077 | 1.000 | 25.68 |
| ATOM | 3367 | CB  | ILE | B | 139 | 45.258 | 34.217 | 68.934 | 1.000 | 29.82 |
| ATOM | 3368 | CG1 | ILE | B | 139 | 46.318 | 34.945 | 68.101 | 1.000 | 41.20 |
| ATOM | 3369 | CD1 | ILE | B | 139 | 47.149 | 35.964 | 68.850 | 1.000 | 20.87 |
| ATOM | 3370 | CG2 | ILE | B | 139 | 45.900 | 33.146 | 69.806 | 1.000 | 14.95 |
| ATOM | 3371 | C   | ILE | B | 139 | 43.126 | 32.902 | 68.985 | 1.000 | 24.46 |
| ATOM | 3372 | O   | ILE | B | 139 | 42.278 | 33.526 | 69.624 | 1.000 | 24.46 |
| ATOM | 3373 | N   | VAL | B | 140 | 43.264 | 31.585 | 69.008 | 1.000 | 19.79 |
| ATOM | 3374 | CA  | VAL | B | 140 | 42.449 | 30.644 | 69.744 | 1.000 | 20.63 |
| ATOM | 3375 | CB  | VAL | B | 140 | 41.747 | 29.622 | 68.832 | 1.000 | 28.33 |
| ATOM | 3376 | CG1 | VAL | B | 140 | 41.044 | 28.585 | 69.698 | 1.000 | 19.08 |
| ATOM | 3377 | CG2 | VAL | B | 140 | 40.773 | 30.296 | 67.875 | 1.000 | 24.28 |
| ATOM | 3378 | C   | VAL | B | 140 | 43.320 | 29.857 | 70.731 | 1.000 | 24.37 |
| ATOM | 3379 | O   | VAL | B | 140 | 44.279 | 29.223 | 70.306 | 1.000 | 18.12 |

**FIGURE 71**

|      |      |     |           |        |        |        |       |       |
|------|------|-----|-----------|--------|--------|--------|-------|-------|
| ATOM | 3380 | N   | MET B 141 | 42.990 | 29.911 | 72.007 | 1.000 | 26.02 |
| ATOM | 3381 | CA  | MET B 141 | 43.681 | 29.264 | 73.114 | 1.000 | 26.63 |
| ATOM | 3382 | CB  | MET B 141 | 44.180 | 30.349 | 74.076 | 1.000 | 21.56 |
| ATOM | 3383 | CG  | MET B 141 | 44.895 | 29.837 | 75.314 | 1.000 | 23.47 |
| ATOM | 3384 | SD  | MET B 141 | 45.830 | 31.148 | 76.140 | 1.000 | 25.00 |
| ATOM | 3385 | CE  | MET B 141 | 46.435 | 30.216 | 77.558 | 1.000 | 23.28 |
| ATOM | 3386 | C   | MET B 141 | 42.749 | 28.270 | 73.801 | 1.000 | 21.18 |
| ATOM | 3387 | O   | MET B 141 | 41.699 | 28.664 | 74.320 | 1.000 | 21.43 |
| ATOM | 3388 | N   | VAL B 142 | 43.079 | 26.991 | 73.799 | 1.000 | 20.95 |
| ATOM | 3389 | CA  | VAL B 142 | 42.221 | 25.959 | 74.364 | 1.000 | 24.30 |
| ATOM | 3390 | CB  | VAL B 142 | 41.813 | 24.856 | 73.371 | 1.000 | 21.57 |
| ATOM | 3391 | CG1 | VAL B 142 | 40.925 | 25.432 | 72.277 | 1.000 | 44.18 |
| ATOM | 3392 | CG2 | VAL B 142 | 43.039 | 24.197 | 72.760 | 1.000 | 32.97 |
| ATOM | 3393 | C   | VAL B 142 | 42.918 | 25.273 | 75.538 | 1.000 | 24.63 |
| ATOM | 3394 | O   | VAL B 142 | 42.870 | 24.057 | 75.706 | 1.000 | 36.20 |
| ATOM | 3395 | N   | THR B 143 | 43.566 | 26.104 | 76.333 | 1.000 | 27.52 |
| ATOM | 3396 | CA  | THR B 143 | 44.179 | 25.667 | 77.575 | 1.000 | 32.61 |
| ATOM | 3397 | CB  | THR B 143 | 45.641 | 25.224 | 77.402 | 1.000 | 33.85 |
| ATOM | 3398 | OG1 | THR B 143 | 46.111 | 24.687 | 78.647 | 1.000 | 32.96 |
| ATOM | 3399 | CG2 | THR B 143 | 46.518 | 26.417 | 77.065 | 1.000 | 21.18 |
| ATOM | 3400 | C   | THR B 143 | 44.152 | 26.815 | 78.577 | 1.000 | 28.98 |
| ATOM | 3401 | O   | THR B 143 | 44.172 | 27.975 | 78.178 | 1.000 | 26.70 |
| ATOM | 3402 | N   | GLN B 144 | 44.115 | 26.478 | 79.855 | 1.000 | 26.36 |
| ATOM | 3403 | CA  | GLN B 144 | 44.388 | 27.496 | 80.868 | 1.000 | 31.26 |
| ATOM | 3404 | CB  | GLN B 144 | 43.644 | 27.201 | 82.158 | 1.000 | 36.91 |
| ATOM | 3405 | CG  | GLN B 144 | 42.161 | 27.541 | 82.146 | 1.000 | 45.71 |
| ATOM | 3406 | CD  | GLN B 144 | 41.465 | 27.010 | 83.387 | 1.000 | 58.10 |
| ATOM | 3407 | OE1 | GLN B 144 | 41.528 | 27.640 | 84.446 | 1.000 | 62.95 |
| ATOM | 3408 | NE2 | GLN B 144 | 40.807 | 25.859 | 83.268 | 1.000 | 68.48 |
| ATOM | 3409 | C   | GLN B 144 | 45.899 | 27.536 | 81.085 | 1.000 | 30.16 |
| ATOM | 3410 | O   | GLN B 144 | 46.586 | 26.558 | 80.764 | 1.000 | 23.48 |
| ATOM | 3411 | N   | CYS B 145 | 46.426 | 28.637 | 81.607 | 1.000 | 23.70 |
| ATOM | 3412 | CA  | CYS B 145 | 47.868 | 28.723 | 81.803 | 1.000 | 23.35 |
| ATOM | 3413 | CB  | CYS B 145 | 48.244 | 30.127 | 82.276 | 1.000 | 17.96 |
| ATOM | 3414 | SG  | CYS B 145 | 48.066 | 31.371 | 80.965 | 1.000 | 36.78 |
| ATOM | 3415 | C   | CYS B 145 | 48.383 | 27.692 | 82.799 | 1.000 | 29.59 |
| ATOM | 3416 | O   | CYS B 145 | 49.493 | 27.168 | 82.657 | 1.000 | 29.74 |
| ATOM | 3417 | N   | VAL B 146 | 47.547 | 27.437 | 83.792 | 1.000 | 26.86 |
| ATOM | 3418 | CA  | VAL B 146 | 47.809 | 26.499 | 84.877 | 1.000 | 25.79 |
| ATOM | 3419 | CB  | VAL B 146 | 48.125 | 27.210 | 86.202 | 1.000 | 30.10 |
| ATOM | 3420 | CG1 | VAL B 146 | 48.824 | 26.274 | 87.179 | 1.000 | 28.99 |
| ATOM | 3421 | CG2 | VAL B 146 | 48.980 | 28.443 | 85.953 | 1.000 | 32.92 |
| ATOM | 3422 | C   | VAL B 146 | 46.606 | 25.573 | 85.059 | 1.000 | 20.95 |
| ATOM | 3423 | O   | VAL B 146 | 45.458 | 25.979 | 85.215 | 1.000 | 28.86 |
| ATOM | 3424 | N   | GLU B 147 | 46.878 | 24.288 | 85.002 | 1.000 | 24.41 |
| ATOM | 3425 | CA  | GLU B 147 | 45.881 | 23.235 | 85.161 | 1.000 | 40.57 |
| ATOM | 3426 | CB  | GLU B 147 | 45.538 | 22.562 | 83.839 | 1.000 | 35.73 |
| ATOM | 3427 | CG  | GLU B 147 | 44.603 | 23.349 | 82.943 | 1.000 | 41.76 |
| ATOM | 3428 | CD  | GLU B 147 | 44.308 | 22.690 | 81.610 | 1.000 | 45.31 |
| ATOM | 3429 | OE1 | GLU B 147 | 44.722 | 21.531 | 81.403 | 1.000 | 43.78 |
| ATOM | 3430 | OE2 | GLU B 147 | 43.653 | 23.322 | 80.749 | 1.000 | 28.21 |
| ATOM | 3431 | C   | GLU B 147 | 46.496 | 22.288 | 86.182 | 1.000 | 45.18 |

**FIGURE 72**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3432 | O   | GLU | B | 147 | 47.457 | 21.558 | 85.926 | 1.000 | 48.42 |
| ATOM | 3433 | N   | LYS | B | 148 | 45.992 | 22.325 | 87.419 | 1.000 | 49.18 |
| ATOM | 3434 | CA  | LYS | B | 148 | 46.881 | 21.658 | 88.390 | 1.000 | 54.02 |
| ATOM | 3435 | CB  | LYS | B | 148 | 46.836 | 22.434 | 89.703 | 1.000 | 46.43 |
| ATOM | 3436 | CG  | LYS | B | 148 | 48.184 | 23.017 | 90.088 | 1.000 | 42.28 |
| ATOM | 3437 | CD  | LYS | B | 148 | 49.019 | 23.482 | 88.921 | 1.000 | 48.15 |
| ATOM | 3438 | CE  | LYS | B | 148 | 50.503 | 23.260 | 89.180 | 1.000 | 46.56 |
| ATOM | 3439 | NZ  | LYS | B | 148 | 51.361 | 24.153 | 88.358 | 1.000 | 39.33 |
| ATOM | 3440 | C   | LYS | B | 148 | 46.554 | 20.182 | 88.515 | 1.000 | 54.15 |
| ATOM | 3441 | O   | LYS | B | 148 | 45.415 | 19.737 | 88.387 | 1.000 | 67.03 |
| ATOM | 3442 | N   | GLY | B | 149 | 47.628 | 19.428 | 88.760 | 1.000 | 52.37 |
| ATOM | 3443 | CA  | GLY | B | 149 | 48.941 | 20.037 | 88.892 | 1.000 | 55.56 |
| ATOM | 3444 | C   | GLY | B | 149 | 49.697 | 20.137 | 87.583 | 1.000 | 63.58 |
| ATOM | 3445 | O   | GLY | B | 149 | 50.182 | 19.100 | 87.123 | 1.000 | 62.06 |
| ATOM | 3446 | N   | ARG | B | 150 | 49.813 | 21.330 | 86.999 | 1.000 | 67.43 |
| ATOM | 3447 | CA  | ARG | B | 150 | 50.589 | 21.516 | 85.780 | 1.000 | 68.36 |
| ATOM | 3448 | CB  | ARG | B | 150 | 50.037 | 20.536 | 84.725 | 1.000 | 77.22 |
| ATOM | 3449 | CG  | ARG | B | 150 | 50.929 | 19.341 | 84.438 | 1.000 | 76.56 |
| ATOM | 3450 | CD  | ARG | B | 150 | 52.223 | 19.406 | 85.233 | 1.000 | 73.15 |
| ATOM | 3451 | NE  | ARG | B | 150 | 53.346 | 19.893 | 84.431 | 1.000 | 71.83 |
| ATOM | 3452 | CZ  | ARG | B | 150 | 54.098 | 19.105 | 83.668 | 1.000 | 75.97 |
| ATOM | 3453 | NH1 | ARG | B | 150 | 53.840 | 17.803 | 83.608 | 1.000 | 77.01 |
| ATOM | 3454 | NH2 | ARG | B | 150 | 55.103 | 19.611 | 82.967 | 1.000 | 68.43 |
| ATOM | 3455 | C   | ARG | B | 150 | 50.600 | 22.925 | 85.204 | 1.000 | 53.31 |
| ATOM | 3456 | O   | ARG | B | 150 | 49.604 | 23.442 | 84.687 | 1.000 | 35.27 |
| ATOM | 3457 | N   | VAL | B | 151 | 51.750 | 23.608 | 85.234 | 1.000 | 34.49 |
| ATOM | 3458 | CA  | VAL | B | 151 | 51.924 | 24.799 | 84.411 | 1.000 | 38.16 |
| ATOM | 3459 | CB  | VAL | B | 151 | 53.297 | 25.469 | 84.557 | 1.000 | 41.62 |
| ATOM | 3460 | CG1 | VAL | B | 151 | 53.498 | 26.491 | 83.437 | 1.000 | 40.64 |
| ATOM | 3461 | CG2 | VAL | B | 151 | 53.471 | 26.163 | 85.899 | 1.000 | 39.00 |
| ATOM | 3462 | C   | VAL | B | 151 | 51.760 | 24.387 | 82.945 | 1.000 | 41.12 |
| ATOM | 3463 | O   | VAL | B | 151 | 52.372 | 23.400 | 82.525 | 1.000 | 39.66 |
| ATOM | 3464 | N   | LYS | B | 152 | 50.959 | 25.079 | 82.142 | 1.000 | 33.45 |
| ATOM | 3465 | CA  | LYS | B | 152 | 50.754 | 24.596 | 80.776 | 1.000 | 28.24 |
| ATOM | 3466 | CB  | LYS | B | 152 | 49.302 | 24.144 | 80.591 | 1.000 | 34.13 |
| ATOM | 3467 | CG  | LYS | B | 152 | 48.830 | 23.155 | 81.645 | 1.000 | 34.20 |
| ATOM | 3468 | CD  | LYS | B | 152 | 49.804 | 22.001 | 81.780 | 1.000 | 38.68 |
| ATOM | 3469 | CE  | LYS | B | 152 | 49.120 | 20.664 | 81.549 | 1.000 | 48.80 |
| ATOM | 3470 | NZ  | LYS | B | 152 | 50.119 | 19.577 | 81.342 | 1.000 | 72.66 |
| ATOM | 3471 | C   | LYS | B | 152 | 51.098 | 25.644 | 79.729 | 1.000 | 31.18 |
| ATOM | 3472 | O   | LYS | B | 152 | 51.407 | 25.310 | 78.584 | 1.000 | 33.64 |
| ATOM | 3473 | N   | CYS | B | 153 | 51.049 | 26.923 | 80.090 | 1.000 | 27.35 |
| ATOM | 3474 | CA  | CYS | B | 153 | 51.346 | 27.960 | 79.093 | 1.000 | 22.51 |
| ATOM | 3475 | CB  | CYS | B | 153 | 50.165 | 28.100 | 78.150 | 1.000 | 16.46 |
| ATOM | 3476 | SG  | CYS | B | 153 | 50.211 | 29.416 | 76.916 | 1.000 | 26.45 |
| ATOM | 3477 | C   | CYS | B | 153 | 51.678 | 29.265 | 79.801 | 1.000 | 31.82 |
| ATOM | 3478 | O   | CYS | B | 153 | 51.084 | 29.606 | 80.822 | 1.000 | 28.53 |
| ATOM | 3479 | N   | ASP | B | 154 | 52.637 | 30.023 | 79.279 | 1.000 | 33.07 |
| ATOM | 3480 | CA  | ASP | B | 154 | 52.907 | 31.332 | 79.858 | 1.000 | 35.38 |
| ATOM | 3481 | CB  | ASP | B | 154 | 54.191 | 31.929 | 79.261 | 1.000 | 35.82 |
| ATOM | 3482 | CG  | ASP | B | 154 | 54.817 | 32.947 | 80.200 | 1.000 | 41.73 |
| ATOM | 3483 | OD1 | ASP | B | 154 | 56.002 | 33.296 | 80.044 | 1.000 | 63.43 |

**FIGURE 73**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3484 | OD2 | ASP | B | 154 | 54.104 | 33.398 | 81.117 | 1.000 | 50.87 |
| ATOM | 3485 | C   | ASP | B | 154 | 51.735 | 32.287 | 79.642 | 1.000 | 41.87 |
| ATOM | 3486 | O   | ASP | B | 154 | 50.951 | 32.111 | 78.703 | 1.000 | 33.32 |
| ATOM | 3487 | N   | HIS | B | 155 | 51.623 | 33.296 | 80.509 | 1.000 | 35.60 |
| ATOM | 3488 | CA  | HIS | B | 155 | 50.654 | 34.375 | 80.304 | 1.000 | 37.44 |
| ATOM | 3489 | CB  | HIS | B | 155 | 50.312 | 35.059 | 81.628 | 1.000 | 36.58 |
| ATOM | 3490 | CG  | HIS | B | 155 | 49.205 | 36.062 | 81.526 | 1.000 | 32.90 |
| ATOM | 3491 | ND1 | HIS | B | 155 | 47.930 | 35.814 | 82.000 | 1.000 | 29.00 |
| ATOM | 3492 | CE1 | HIS | B | 155 | 47.168 | 36.872 | 81.774 | 1.000 | 30.32 |
| ATOM | 3493 | NE2 | HIS | B | 155 | 47.903 | 37.796 | 81.172 | 1.000 | 34.71 |
| ATOM | 3494 | CD2 | HIS | B | 155 | 49.182 | 37.312 | 81.009 | 1.000 | 27.70 |
| ATOM | 3495 | C   | HIS | B | 155 | 51.236 | 35.374 | 79.311 | 1.000 | 36.71 |
| ATOM | 3496 | O   | HIS | B | 155 | 51.750 | 36.422 | 79.691 | 1.000 | 42.00 |
| ATOM | 3497 | N   | TYR | B | 156 | 51.192 | 35.068 | 78.016 | 1.000 | 29.11 |
| ATOM | 3498 | CA  | TYR | B | 156 | 52.011 | 35.820 | 77.081 | 1.000 | 24.84 |
| ATOM | 3499 | CB  | TYR | B | 156 | 52.303 | 34.932 | 75.855 | 1.000 | 27.19 |
| ATOM | 3500 | CG  | TYR | B | 156 | 51.050 | 34.394 | 75.208 | 1.000 | 24.09 |
| ATOM | 3501 | CD1 | TYR | B | 156 | 50.488 | 35.051 | 74.120 | 1.000 | 16.98 |
| ATOM | 3502 | CE1 | TYR | B | 156 | 49.344 | 34.554 | 73.528 | 1.000 | 17.14 |
| ATOM | 3503 | CZ  | TYR | B | 156 | 48.745 | 33.407 | 73.996 | 1.000 | 25.77 |
| ATOM | 3504 | OH  | TYR | B | 156 | 47.596 | 32.928 | 73.387 | 1.000 | 23.27 |
| ATOM | 3505 | CE2 | TYR | B | 156 | 49.294 | 32.745 | 75.074 | 1.000 | 27.41 |
| ATOM | 3506 | CD2 | TYR | B | 156 | 50.439 | 33.238 | 75.672 | 1.000 | 27.13 |
| ATOM | 3507 | C   | TYR | B | 156 | 51.409 | 37.129 | 76.615 | 1.000 | 23.96 |
| ATOM | 3508 | O   | TYR | B | 156 | 51.948 | 37.722 | 75.673 | 1.000 | 30.34 |
| ATOM | 3509 | N   | TRP | B | 157 | 50.332 | 37.596 | 77.228 | 1.000 | 29.38 |
| ATOM | 3510 | CA  | TRP | B | 157 | 49.801 | 38.920 | 76.885 | 1.000 | 30.99 |
| ATOM | 3511 | CB  | TRP | B | 157 | 48.389 | 38.798 | 76.324 | 1.000 | 35.30 |
| ATOM | 3512 | CG  | TRP | B | 157 | 47.436 | 38.178 | 77.304 | 1.000 | 37.36 |
| ATOM | 3513 | CD1 | TRP | B | 157 | 46.608 | 38.819 | 78.180 | 1.000 | 32.25 |
| ATOM | 3514 | NE1 | TRP | B | 157 | 45.897 | 37.886 | 78.896 | 1.000 | 33.37 |
| ATOM | 3515 | CE2 | TRP | B | 157 | 46.257 | 36.626 | 78.495 | 1.000 | 24.24 |
| ATOM | 3516 | CD2 | TRP | B | 157 | 47.227 | 36.772 | 77.488 | 1.000 | 31.89 |
| ATOM | 3517 | CE3 | TRP | B | 157 | 47.774 | 35.630 | 76.894 | 1.000 | 32.73 |
| ATOM | 3518 | CZ3 | TRP | B | 157 | 47.334 | 34.394 | 77.324 | 1.000 | 31.61 |
| ATOM | 3519 | CH2 | TRP | B | 157 | 46.366 | 34.269 | 78.328 | 1.000 | 31.07 |
| ATOM | 3520 | CZ2 | TRP | B | 157 | 45.819 | 35.378 | 78.923 | 1.000 | 30.59 |
| ATOM | 3521 | C   | TRP | B | 157 | 49.806 | 39.815 | 78.116 | 1.000 | 33.23 |
| ATOM | 3522 | O   | TRP | B | 157 | 50.003 | 39.308 | 79.229 | 1.000 | 47.58 |
| ATOM | 3523 | N   | PRO | B | 158 | 49.613 | 41.119 | 77.999 | 1.000 | 35.32 |
| ATOM | 3524 | CA  | PRO | B | 158 | 49.665 | 41.957 | 79.206 | 1.000 | 42.97 |
| ATOM | 3525 | CB  | PRO | B | 158 | 49.605 | 43.384 | 78.670 | 1.000 | 36.94 |
| ATOM | 3526 | CG  | PRO | B | 158 | 49.779 | 43.296 | 77.200 | 1.000 | 32.51 |
| ATOM | 3527 | CD  | PRO | B | 158 | 49.347 | 41.916 | 76.793 | 1.000 | 36.20 |
| ATOM | 3528 | C   | PRO | B | 158 | 48.468 | 41.701 | 80.128 | 1.000 | 58.41 |
| ATOM | 3529 | O   | PRO | B | 158 | 47.343 | 41.559 | 79.645 | 1.000 | 65.51 |
| ATOM | 3530 | N   | ALA | B | 159 | 48.739 | 41.658 | 81.422 | 1.000 | 68.74 |
| ATOM | 3531 | CA  | ALA | B | 159 | 47.823 | 41.404 | 82.518 | 1.000 | 64.94 |
| ATOM | 3532 | CB  | ALA | B | 159 | 48.387 | 41.972 | 83.819 | 1.000 | 34.74 |
| ATOM | 3533 | C   | ALA | B | 159 | 46.428 | 41.975 | 82.282 | 1.000 | 65.31 |
| ATOM | 3534 | O   | ALA | B | 159 | 45.468 | 41.222 | 82.121 | 1.000 | 68.71 |
| ATOM | 3535 | N   | ASP | B | 160 | 46.330 | 43.297 | 82.278 | 1.000 | 66.84 |

**FIGURE 74**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3536 | CA  | ASP | B | 160 | 45.079 | 44.010 | 82.063 | 1.000 | 69.30 |
| ATOM | 3537 | CB  | ASP | B | 160 | 44.668 | 44.824 | 83.286 | 1.000 | 73.78 |
| ATOM | 3538 | CG  | ASP | B | 160 | 45.671 | 44.813 | 84.417 | 1.000 | 78.54 |
| ATOM | 3539 | OD1 | ASP | B | 160 | 46.696 | 45.535 | 84.324 | 1.000 | 85.06 |
| ATOM | 3540 | OD2 | ASP | B | 160 | 45.449 | 44.083 | 85.410 | 1.000 | 82.66 |
| ATOM | 3541 | C   | ASP | B | 160 | 45.199 | 44.934 | 80.850 | 1.000 | 70.60 |
| ATOM | 3542 | O   | ASP | B | 160 | 45.922 | 44.612 | 79.904 | 1.000 | 80.81 |
| ATOM | 3543 | N   | GLN | B | 161 | 44.503 | 46.063 | 80.897 | 1.000 | 65.68 |
| ATOM | 3544 | CA  | GLN | B | 161 | 44.460 | 47.034 | 79.813 | 1.000 | 60.98 |
| ATOM | 3545 | CB  | GLN | B | 161 | 43.341 | 48.054 | 80.079 | 1.000 | 66.64 |
| ATOM | 3546 | CG  | GLN | B | 161 | 41.977 | 47.435 | 80.326 | 1.000 | 70.82 |
| ATOM | 3547 | CD  | GLN | B | 161 | 41.431 | 46.682 | 79.129 | 1.000 | 73.10 |
| ATOM | 3548 | OE1 | GLN | B | 161 | 41.858 | 46.906 | 77.995 | 1.000 | 91.18 |
| ATOM | 3549 | NE2 | GLN | B | 161 | 40.481 | 45.781 | 79.367 | 1.000 | 51.42 |
| ATOM | 3550 | C   | GLN | B | 161 | 45.774 | 47.770 | 79.607 | 1.000 | 52.94 |
| ATOM | 3551 | O   | GLN | B | 161 | 45.860 | 48.713 | 78.819 | 1.000 | 46.56 |
| ATOM | 3552 | N   | ASP | B | 162 | 46.841 | 47.376 | 80.294 | 1.000 | 57.53 |
| ATOM | 3553 | CA  | ASP | B | 162 | 48.126 | 48.048 | 80.111 | 1.000 | 53.21 |
| ATOM | 3554 | CB  | ASP | B | 162 | 49.080 | 47.691 | 81.251 | 1.000 | 60.81 |
| ATOM | 3555 | CG  | ASP | B | 162 | 49.331 | 46.204 | 81.393 | 1.000 | 64.03 |
| ATOM | 3556 | OD1 | ASP | B | 162 | 48.588 | 45.415 | 80.770 | 1.000 | 73.29 |
| ATOM | 3557 | OD2 | ASP | B | 162 | 50.272 | 45.829 | 82.129 | 1.000 | 52.70 |
| ATOM | 3558 | C   | ASP | B | 162 | 48.742 | 47.700 | 78.759 | 1.000 | 46.46 |
| ATOM | 3559 | O   | ASP | B | 162 | 48.083 | 47.149 | 77.874 | 1.000 | 52.43 |
| ATOM | 3560 | N   | SER | B | 163 | 50.014 | 48.039 | 78.604 | 1.000 | 36.08 |
| ATOM | 3561 | CA  | SER | B | 163 | 50.763 | 47.761 | 77.385 | 1.000 | 30.11 |
| ATOM | 3562 | CB  | SER | B | 163 | 50.905 | 49.014 | 76.523 | 1.000 | 37.96 |
| ATOM | 3563 | OG  | SER | B | 163 | 51.383 | 50.101 | 77.295 | 1.000 | 38.12 |
| ATOM | 3564 | C   | SER | B | 163 | 52.141 | 47.223 | 77.724 | 1.000 | 31.57 |
| ATOM | 3565 | O   | SER | B | 163 | 52.646 | 47.355 | 78.838 | 1.000 | 35.55 |
| ATOM | 3566 | N   | LEU | B | 164 | 52.776 | 46.591 | 76.741 | 1.000 | 30.19 |
| ATOM | 3567 | CA  | LEU | B | 164 | 54.081 | 46.002 | 77.023 | 1.000 | 21.86 |
| ATOM | 3568 | CB  | LEU | B | 164 | 53.918 | 44.691 | 77.779 | 1.000 | 37.42 |
| ATOM | 3569 | CG  | LEU | B | 164 | 53.641 | 44.732 | 79.281 | 1.000 | 38.91 |
| ATOM | 3570 | CD1 | LEU | B | 164 | 53.495 | 43.319 | 79.843 | 1.000 | 28.89 |
| ATOM | 3571 | CD2 | LEU | B | 164 | 54.736 | 45.470 | 80.031 | 1.000 | 42.72 |
| ATOM | 3572 | C   | LEU | B | 164 | 54.822 | 45.780 | 75.715 | 1.000 | 27.76 |
| ATOM | 3573 | O   | LEU | B | 164 | 54.201 | 45.635 | 74.660 | 1.000 | 28.16 |
| ATOM | 3574 | N   | TYR | B | 165 | 56.150 | 45.767 | 75.799 | 1.000 | 29.39 |
| ATOM | 3575 | CA  | TYR | B | 165 | 56.959 | 45.469 | 74.631 | 1.000 | 27.11 |
| ATOM | 3576 | CB  | TYR | B | 165 | 58.338 | 46.113 | 74.728 | 1.000 | 24.50 |
| ATOM | 3577 | CG  | TYR | B | 165 | 58.373 | 47.576 | 74.362 | 1.000 | 33.29 |
| ATOM | 3578 | CD1 | TYR | B | 165 | 58.505 | 47.926 | 73.022 | 1.000 | 27.89 |
| ATOM | 3579 | CE1 | TYR | B | 165 | 58.538 | 49.248 | 72.635 | 1.000 | 31.36 |
| ATOM | 3580 | CZ  | TYR | B | 165 | 58.443 | 50.244 | 73.581 | 1.000 | 24.85 |
| ATOM | 3581 | OH  | TYR | B | 165 | 58.487 | 51.546 | 73.139 | 1.000 | 26.61 |
| ATOM | 3582 | CE2 | TYR | B | 165 | 58.309 | 49.930 | 74.915 | 1.000 | 28.53 |
| ATOM | 3583 | CD2 | TYR | B | 165 | 58.271 | 48.594 | 75.307 | 1.000 | 28.19 |
| ATOM | 3584 | C   | TYR | B | 165 | 57.109 | 43.955 | 74.503 | 1.000 | 32.17 |
| ATOM | 3585 | O   | TYR | B | 165 | 57.195 | 43.254 | 75.511 | 1.000 | 29.95 |
| ATOM | 3586 | N   | TYR | B | 166 | 57.152 | 43.472 | 73.271 | 1.000 | 28.70 |
| ATOM | 3587 | CA  | TYR | B | 166 | 57.498 | 42.072 | 73.035 | 1.000 | 27.96 |

**FIGURE 75**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3588 | CB  | TYR | B | 166 | 56.268 | 41.232 | 72.710 | 1.000 | 29.27 |
| ATOM | 3589 | CG  | TYR | B | 166 | 55.350 | 41.031 | 73.899 | 1.000 | 32.16 |
| ATOM | 3590 | CD1 | TYR | B | 166 | 55.542 | 39.987 | 74.805 | 1.000 | 27.15 |
| ATOM | 3591 | CE1 | TYR | B | 166 | 54.689 | 39.821 | 75.884 | 1.000 | 26.48 |
| ATOM | 3592 | CZ  | TYR | B | 166 | 53.637 | 40.699 | 76.065 | 1.000 | 31.42 |
| ATOM | 3593 | OH  | TYR | B | 166 | 52.780 | 40.552 | 77.133 | 1.000 | 26.92 |
| ATOM | 3594 | CE2 | TYR | B | 166 | 53.427 | 41.738 | 75.182 | 1.000 | 25.16 |
| ATOM | 3595 | CD2 | TYR | B | 166 | 54.282 | 41.897 | 74.107 | 1.000 | 30.85 |
| ATOM | 3596 | C   | TYR | B | 166 | 58.533 | 42.065 | 71.926 | 1.000 | 23.40 |
| ATOM | 3597 | O   | TYR | B | 166 | 58.221 | 42.038 | 70.746 | 1.000 | 29.44 |
| ATOM | 3598 | N   | GLY | B | 167 | 59.815 | 42.124 | 72.303 | 1.000 | 30.73 |
| ATOM | 3599 | CA  | GLY | B | 167 | 60.795 | 42.293 | 71.225 | 1.000 | 31.29 |
| ATOM | 3600 | C   | GLY | B | 167 | 60.629 | 43.677 | 70.620 | 1.000 | 34.66 |
| ATOM | 3601 | O   | GLY | B | 167 | 60.636 | 44.683 | 71.340 | 1.000 | 26.60 |
| ATOM | 3602 | N   | ASP | B | 168 | 60.475 | 43.757 | 69.302 | 1.000 | 29.65 |
| ATOM | 3603 | CA  | ASP | B | 168 | 60.388 | 45.070 | 68.660 | 1.000 | 31.97 |
| ATOM | 3604 | CB  | ASP | B | 168 | 61.050 | 45.062 | 67.282 | 1.000 | 30.77 |
| ATOM | 3605 | CG  | ASP | B | 168 | 62.559 | 44.932 | 67.417 | 1.000 | 44.29 |
| ATOM | 3606 | OD1 | ASP | B | 168 | 63.059 | 45.103 | 68.550 | 1.000 | 70.44 |
| ATOM | 3607 | OD2 | ASP | B | 168 | 63.238 | 44.655 | 66.411 | 1.000 | 63.44 |
| ATOM | 3608 | C   | ASP | B | 168 | 58.935 | 45.510 | 68.551 | 1.000 | 32.07 |
| ATOM | 3609 | O   | ASP | B | 168 | 58.619 | 46.594 | 68.076 | 1.000 | 32.90 |
| ATOM | 3610 | N   | LEU | B | 169 | 58.073 | 44.613 | 69.025 | 1.000 | 29.35 |
| ATOM | 3611 | CA  | LEU | B | 169 | 56.648 | 44.870 | 68.984 | 1.000 | 33.24 |
| ATOM | 3612 | CB  | LEU | B | 169 | 55.877 | 43.576 | 68.686 | 1.000 | 30.90 |
| ATOM | 3613 | CG  | LEU | B | 169 | 56.205 | 42.932 | 67.336 | 1.000 | 32.40 |
| ATOM | 3614 | CD1 | LEU | B | 169 | 55.292 | 41.738 | 67.129 | 1.000 | 26.83 |
| ATOM | 3615 | CD2 | LEU | B | 169 | 56.082 | 43.955 | 66.219 | 1.000 | 27.58 |
| ATOM | 3616 | C   | LEU | B | 169 | 56.111 | 45.433 | 70.294 | 1.000 | 32.00 |
| ATOM | 3617 | O   | LEU | B | 169 | 56.642 | 45.147 | 71.365 | 1.000 | 27.18 |
| ATOM | 3618 | N   | ILE | B | 170 | 55.042 | 46.205 | 70.127 | 1.000 | 23.43 |
| ATOM | 3619 | CA  | ILE | B | 170 | 54.297 | 46.711 | 71.263 | 1.000 | 37.97 |
| ATOM | 3620 | CB  | ILE | B | 170 | 54.333 | 48.242 | 71.369 | 1.000 | 44.96 |
| ATOM | 3621 | CG1 | ILE | B | 170 | 53.206 | 48.832 | 72.219 | 1.000 | 51.13 |
| ATOM | 3622 | CD1 | ILE | B | 170 | 53.662 | 49.989 | 73.089 | 1.000 | 79.46 |
| ATOM | 3623 | CG2 | ILE | B | 170 | 54.345 | 48.876 | 69.991 | 1.000 | 56.59 |
| ATOM | 3624 | C   | ILE | B | 170 | 52.851 | 46.228 | 71.147 | 1.000 | 36.98 |
| ATOM | 3625 | O   | ILE | B | 170 | 52.247 | 46.337 | 70.083 | 1.000 | 29.48 |
| ATOM | 3626 | N   | LEU | B | 171 | 52.367 | 45.700 | 72.258 | 1.000 | 37.92 |
| ATOM | 3627 | CA  | LEU | B | 171 | 51.015 | 45.200 | 72.405 | 1.000 | 39.12 |
| ATOM | 3628 | CB  | LEU | B | 171 | 51.037 | 43.709 | 72.767 | 1.000 | 46.39 |
| ATOM | 3629 | CG  | LEU | B | 171 | 50.043 | 42.860 | 71.971 | 1.000 | 52.95 |
| ATOM | 3630 | CD1 | LEU | B | 171 | 50.694 | 41.558 | 71.563 | 1.000 | 42.82 |
| ATOM | 3631 | CD2 | LEU | B | 171 | 48.783 | 42.619 | 72.784 | 1.000 | 80.84 |
| ATOM | 3632 | C   | LEU | B | 171 | 50.235 | 45.939 | 73.482 | 1.000 | 37.92 |
| ATOM | 3633 | O   | LEU | B | 171 | 50.744 | 46.261 | 74.556 | 1.000 | 41.84 |
| ATOM | 3634 | N   | GLN | B | 172 | 48.962 | 46.207 | 73.191 | 1.000 | 33.26 |
| ATOM | 3635 | CA  | GLN | B | 172 | 48.132 | 46.767 | 74.257 | 1.000 | 42.90 |
| ATOM | 3636 | CB  | GLN | B | 172 | 47.929 | 48.272 | 74.095 | 1.000 | 43.81 |
| ATOM | 3637 | CG  | GLN | B | 172 | 46.841 | 48.669 | 73.123 | 1.000 | 44.65 |
| ATOM | 3638 | CD  | GLN | B | 172 | 46.760 | 50.170 | 72.905 | 1.000 | 41.71 |
| ATOM | 3639 | OE1 | GLN | B | 172 | 47.004 | 50.675 | 71.809 | 1.000 | 39.38 |

**FIGURE 76**



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3640 | NE2 | GLN | B | 172 | 46.410 | 50.886 | 73.963 | 1.000 | 51.04 |
| ATOM | 3641 | C   | GLN | B | 172 | 46.800 | 46.028 | 74.274 | 1.000 | 36.46 |
| ATOM | 3642 | O   | GLN | B | 172 | 46.205 | 45.820 | 73.214 | 1.000 | 30.33 |
| ATOM | 3643 | N   | MET | B | 173 | 46.349 | 45.629 | 75.460 | 1.000 | 34.57 |
| ATOM | 3644 | CA  | MET | B | 173 | 45.024 | 45.020 | 75.526 | 1.000 | 37.82 |
| ATOM | 3645 | CB  | MET | B | 173 | 44.827 | 44.177 | 76.786 | 1.000 | 44.70 |
| ATOM | 3646 | CG  | MET | B | 173 | 43.371 | 44.165 | 77.243 | 1.000 | 48.88 |
| ATOM | 3647 | SD  | MET | B | 173 | 43.091 | 43.051 | 78.637 | 1.000 | 61.82 |
| ATOM | 3648 | CE  | MET | B | 173 | 43.023 | 41.490 | 77.765 | 1.000 | 30.24 |
| ATOM | 3649 | C   | MET | B | 173 | 43.960 | 46.115 | 75.496 | 1.000 | 37.98 |
| ATOM | 3650 | O   | MET | B | 173 | 43.913 | 46.968 | 76.387 | 1.000 | 50.74 |
| ATOM | 3651 | N   | LEU | B | 174 | 43.116 | 46.087 | 74.476 | 1.000 | 39.28 |
| ATOM | 3652 | CA  | LEU | B | 174 | 42.041 | 47.069 | 74.379 | 1.000 | 40.72 |
| ATOM | 3653 | CB  | LEU | B | 174 | 41.705 | 47.353 | 72.911 | 1.000 | 40.97 |
| ATOM | 3654 | CG  | LEU | B | 174 | 42.894 | 47.860 | 72.084 | 1.000 | 48.67 |
| ATOM | 3655 | CD1 | LEU | B | 174 | 42.466 | 48.190 | 70.666 | 1.000 | 63.07 |
| ATOM | 3656 | CD2 | LEU | B | 174 | 43.524 | 49.058 | 72.778 | 1.000 | 40.09 |
| ATOM | 3657 | C   | LEU | B | 174 | 40.794 | 46.608 | 75.113 | 1.000 | 37.13 |
| ATOM | 3658 | O   | LEU | B | 174 | 39.994 | 47.450 | 75.515 | 1.000 | 41.98 |
| ATOM | 3659 | N   | SER | B | 175 | 40.613 | 45.295 | 75.288 | 1.000 | 36.81 |
| ATOM | 3660 | CA  | SER | B | 175 | 39.379 | 44.856 | 75.936 | 1.000 | 37.02 |
| ATOM | 3661 | CB  | SER | B | 175 | 38.204 | 45.077 | 74.978 | 1.000 | 39.53 |
| ATOM | 3662 | OG  | SER | B | 175 | 38.164 | 44.075 | 73.975 | 1.000 | 60.16 |
| ATOM | 3663 | C   | SER | B | 175 | 39.419 | 43.397 | 76.372 | 1.000 | 43.07 |
| ATOM | 3664 | O   | SER | B | 175 | 40.144 | 42.583 | 75.801 | 1.000 | 35.52 |
| ATOM | 3665 | N   | GLU | B | 176 | 38.616 | 43.077 | 77.387 | 1.000 | 36.53 |
| ATOM | 3666 | CA  | GLU | B | 176 | 38.525 | 41.721 | 77.899 | 1.000 | 37.42 |
| ATOM | 3667 | CB  | GLU | B | 176 | 39.524 | 41.528 | 79.050 | 1.000 | 29.90 |
| ATOM | 3668 | CG  | GLU | B | 176 | 39.524 | 40.101 | 79.570 | 1.000 | 36.55 |
| ATOM | 3669 | CD  | GLU | B | 176 | 40.377 | 39.924 | 80.806 | 1.000 | 41.20 |
| ATOM | 3670 | OE1 | GLU | B | 176 | 39.808 | 39.980 | 81.913 | 1.000 | 65.49 |
| ATOM | 3671 | OE2 | GLU | B | 176 | 41.602 | 39.726 | 80.667 | 1.000 | 51.95 |
| ATOM | 3672 | C   | GLU | B | 176 | 37.120 | 41.366 | 78.371 | 1.000 | 42.69 |
| ATOM | 3673 | O   | GLU | B | 176 | 36.658 | 41.868 | 79.400 | 1.000 | 44.27 |
| ATOM | 3674 | N   | SER | B | 177 | 36.434 | 40.496 | 77.627 | 1.000 | 39.90 |
| ATOM | 3675 | CA  | SER | B | 177 | 35.073 | 40.107 | 77.983 | 1.000 | 35.04 |
| ATOM | 3676 | CB  | SER | B | 177 | 34.101 | 40.295 | 76.816 | 1.000 | 36.67 |
| ATOM | 3677 | OG  | SER | B | 177 | 34.475 | 41.395 | 76.007 | 1.000 | 52.82 |
| ATOM | 3678 | C   | SER | B | 177 | 35.030 | 38.658 | 78.448 | 1.000 | 41.90 |
| ATOM | 3679 | O   | SER | B | 177 | 35.160 | 37.715 | 77.669 | 1.000 | 42.75 |
| ATOM | 3680 | N   | VAL | B | 178 | 34.840 | 38.482 | 79.750 | 1.000 | 40.45 |
| ATOM | 3681 | CA  | VAL | B | 178 | 34.819 | 37.128 | 80.295 | 1.000 | 49.91 |
| ATOM | 3682 | CB  | VAL | B | 178 | 35.272 | 37.144 | 81.768 | 1.000 | 56.06 |
| ATOM | 3683 | CG1 | VAL | B | 178 | 35.518 | 35.735 | 82.276 | 1.000 | 36.78 |
| ATOM | 3684 | CG2 | VAL | B | 178 | 36.520 | 38.006 | 81.909 | 1.000 | 58.94 |
| ATOM | 3685 | C   | VAL | B | 178 | 33.439 | 36.509 | 80.163 | 1.000 | 50.01 |
| ATOM | 3686 | O   | VAL | B | 178 | 32.445 | 37.037 | 80.659 | 1.000 | 63.04 |
| ATOM | 3687 | N   | LEU | B | 179 | 33.372 | 35.372 | 79.478 | 1.000 | 45.68 |
| ATOM | 3688 | CA  | LEU | B | 179 | 32.098 | 34.653 | 79.362 | 1.000 | 38.65 |
| ATOM | 3689 | CB  | LEU | B | 179 | 31.753 | 34.401 | 77.900 | 1.000 | 37.56 |
| ATOM | 3690 | CG  | LEU | B | 179 | 30.892 | 35.472 | 77.222 | 1.000 | 42.61 |
| ATOM | 3691 | CD1 | LEU | B | 179 | 30.991 | 36.805 | 77.946 | 1.000 | 33.74 |

**FIGURE 77**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3692 | CD2 | LEU | B | 179 | 31.286 | 35.631 | 75.766 | 1.000 | 47.05 |
| ATOM | 3693 | C   | LEU | B | 179 | 32.206 | 33.383 | 80.189 | 1.000 | 30.01 |
| ATOM | 3694 | O   | LEU | B | 179 | 33.317 | 33.035 | 80.611 | 1.000 | 33.11 |
| ATOM | 3695 | N   | PRO | B | 180 | 31.108 | 32.694 | 80.467 | 1.000 | 44.43 |
| ATOM | 3696 | CA  | PRO | B | 180 | 31.210 | 31.516 | 81.345 | 1.000 | 49.89 |
| ATOM | 3697 | CB  | PRO | B | 180 | 29.766 | 31.004 | 81.441 | 1.000 | 47.48 |
| ATOM | 3698 | CG  | PRO | B | 180 | 28.932 | 32.194 | 81.096 | 1.000 | 47.96 |
| ATOM | 3699 | CD  | PRO | B | 180 | 29.720 | 32.929 | 80.038 | 1.000 | 48.96 |
| ATOM | 3700 | C   | PRO | B | 180 | 32.130 | 30.439 | 80.793 | 1.000 | 43.82 |
| ATOM | 3701 | O   | PRO | B | 180 | 32.877 | 29.834 | 81.569 | 1.000 | 44.36 |
| ATOM | 3702 | N   | GLU | B | 181 | 32.144 | 30.139 | 79.492 | 1.000 | 42.02 |
| ATOM | 3703 | CA  | GLU | B | 181 | 33.041 | 29.044 | 79.095 | 1.000 | 41.65 |
| ATOM | 3704 | CB  | GLU | B | 181 | 32.305 | 28.017 | 78.245 | 1.000 | 42.17 |
| ATOM | 3705 | CG  | GLU | B | 181 | 31.191 | 27.274 | 78.964 | 1.000 | 46.96 |
| ATOM | 3706 | CD  | GLU | B | 181 | 30.000 | 27.055 | 78.047 | 1.000 | 47.94 |
| ATOM | 3707 | OE1 | GLU | B | 181 | 29.114 | 27.932 | 78.017 | 1.000 | 66.99 |
| ATOM | 3708 | OE2 | GLU | B | 181 | 29.958 | 26.017 | 77.358 | 1.000 | 66.16 |
| ATOM | 3709 | C   | GLU | B | 181 | 34.270 | 29.552 | 78.353 | 1.000 | 42.89 |
| ATOM | 3710 | O   | GLU | B | 181 | 35.211 | 28.790 | 78.114 | 1.000 | 45.33 |
| ATOM | 3711 | N   | TRP | B | 182 | 34.287 | 30.831 | 77.987 | 1.000 | 38.96 |
| ATOM | 3712 | CA  | TRP | B | 182 | 35.473 | 31.378 | 77.343 | 1.000 | 34.57 |
| ATOM | 3713 | CB  | TRP | B | 182 | 35.493 | 31.021 | 75.853 | 1.000 | 34.24 |
| ATOM | 3714 | CG  | TRP | B | 182 | 34.289 | 31.453 | 75.078 | 1.000 | 31.49 |
| ATOM | 3715 | CD1 | TRP | B | 182 | 34.055 | 32.679 | 74.531 | 1.000 | 33.21 |
| ATOM | 3716 | NE1 | TRP | B | 182 | 32.839 | 32.683 | 73.891 | 1.000 | 30.07 |
| ATOM | 3717 | CE2 | TRP | B | 182 | 32.258 | 31.451 | 74.014 | 1.000 | 24.47 |
| ATOM | 3718 | CD2 | TRP | B | 182 | 33.145 | 30.644 | 74.755 | 1.000 | 36.54 |
| ATOM | 3719 | CE3 | TRP | B | 182 | 32.793 | 29.317 | 75.030 | 1.000 | 38.44 |
| ATOM | 3720 | CZ3 | TRP | B | 182 | 31.582 | 28.837 | 74.562 | 1.000 | 36.86 |
| ATOM | 3721 | CH2 | TRP | B | 182 | 30.725 | 29.670 | 73.827 | 1.000 | 32.83 |
| ATOM | 3722 | CZ2 | TRP | B | 182 | 31.038 | 30.971 | 73.543 | 1.000 | 25.32 |
| ATOM | 3723 | C   | TRP | B | 182 | 35.581 | 32.890 | 77.481 | 1.000 | 29.73 |
| ATOM | 3724 | O   | TRP | B | 182 | 34.637 | 33.609 | 77.802 | 1.000 | 34.04 |
| ATOM | 3725 | N   | THR | B | 183 | 36.786 | 33.370 | 77.203 | 1.000 | 19.61 |
| ATOM | 3726 | CA  | THR | B | 183 | 37.043 | 34.808 | 77.245 | 1.000 | 24.25 |
| ATOM | 3727 | CB  | THR | B | 183 | 38.106 | 35.096 | 78.329 | 1.000 | 27.46 |
| ATOM | 3728 | OG1 | THR | B | 183 | 37.562 | 34.709 | 79.589 | 1.000 | 35.93 |
| ATOM | 3729 | CG2 | THR | B | 183 | 38.446 | 36.570 | 78.408 | 1.000 | 27.17 |
| ATOM | 3730 | C   | THR | B | 183 | 37.539 | 35.333 | 75.910 | 1.000 | 20.91 |
| ATOM | 3731 | O   | THR | B | 183 | 38.454 | 34.749 | 75.312 | 1.000 | 28.00 |
| ATOM | 3732 | N   | ILE | B | 184 | 36.966 | 36.423 | 75.422 | 1.000 | 26.34 |
| ATOM | 3733 | CA  | ILE | B | 184 | 37.472 | 37.068 | 74.208 | 1.000 | 26.11 |
| ATOM | 3734 | CB  | ILE | B | 184 | 36.341 | 37.420 | 73.235 | 1.000 | 29.02 |
| ATOM | 3735 | CG1 | ILE | B | 184 | 35.592 | 36.198 | 72.681 | 1.000 | 36.60 |
| ATOM | 3736 | CD1 | ILE | B | 184 | 34.154 | 36.545 | 72.341 | 1.000 | 36.57 |
| ATOM | 3737 | CG2 | ILE | B | 184 | 36.819 | 38.293 | 72.087 | 1.000 | 18.36 |
| ATOM | 3738 | C   | ILE | B | 184 | 38.232 | 38.333 | 74.580 | 1.000 | 31.53 |
| ATOM | 3739 | O   | ILE | B | 184 | 37.781 | 39.186 | 75.345 | 1.000 | 38.29 |
| ATOM | 3740 | N   | ARG | B | 185 | 39.437 | 38.501 | 74.043 | 1.000 | 34.57 |
| ATOM | 3741 | CA  | ARG | B | 185 | 40.147 | 39.754 | 74.292 | 1.000 | 25.10 |
| ATOM | 3742 | CB  | ARG | B | 185 | 41.417 | 39.538 | 75.100 | 1.000 | 28.99 |
| ATOM | 3743 | CG  | ARG | B | 185 | 41.209 | 39.034 | 76.522 | 1.000 | 31.53 |

**FIGURE 78**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3744 | CD  | ARG | B | 185 | 42.403 | 38.222 | 76.976 | 1.000 | 25.65 |
| ATOM | 3745 | NE  | ARG | B | 185 | 42.343 | 37.791 | 78.364 | 1.000 | 21.83 |
| ATOM | 3746 | CZ  | ARG | B | 185 | 42.092 | 36.551 | 78.753 | 1.000 | 23.41 |
| ATOM | 3747 | NH1 | ARG | B | 185 | 41.864 | 35.591 | 77.867 | 1.000 | 20.48 |
| ATOM | 3748 | NH2 | ARG | B | 185 | 42.064 | 36.264 | 80.047 | 1.000 | 23.08 |
| ATOM | 3749 | C   | ARG | B | 185 | 40.474 | 40.399 | 72.952 | 1.000 | 34.69 |
| ATOM | 3750 | O   | ARG | B | 185 | 40.557 | 39.744 | 71.909 | 1.000 | 35.97 |
| ATOM | 3751 | N   | GLU | B | 186 | 40.657 | 41.714 | 72.993 | 1.000 | 27.86 |
| ATOM | 3752 | CA  | GLU | B | 186 | 41.104 | 42.376 | 71.771 | 1.000 | 30.56 |
| ATOM | 3753 | CB  | GLU | B | 186 | 40.003 | 43.261 | 71.200 | 1.000 | 27.97 |
| ATOM | 3754 | CG  | GLU | B | 186 | 38.651 | 42.555 | 71.232 | 1.000 | 39.02 |
| ATOM | 3755 | CD  | GLU | B | 186 | 37.530 | 43.456 | 70.746 | 1.000 | 52.48 |
| ATOM | 3756 | OE1 | GLU | B | 186 | 37.819 | 44.357 | 69.928 | 1.000 | 68.25 |
| ATOM | 3757 | OE2 | GLU | B | 186 | 36.378 | 43.243 | 71.180 | 1.000 | 77.37 |
| ATOM | 3758 | C   | GLU | B | 186 | 42.373 | 43.152 | 72.110 | 1.000 | 32.85 |
| ATOM | 3759 | O   | GLU | B | 186 | 42.405 | 43.798 | 73.154 | 1.000 | 31.08 |
| ATOM | 3760 | N   | PHE | B | 187 | 43.349 | 43.031 | 71.236 | 1.000 | 30.67 |
| ATOM | 3761 | CA  | PHE | B | 187 | 44.651 | 43.643 | 71.332 | 1.000 | 28.22 |
| ATOM | 3762 | CB  | PHE | B | 187 | 45.761 | 42.599 | 71.472 | 1.000 | 23.26 |
| ATOM | 3763 | CG  | PHE | B | 187 | 45.580 | 41.563 | 72.546 | 1.000 | 30.99 |
| ATOM | 3764 | CD1 | PHE | B | 187 | 45.238 | 40.260 | 72.244 | 1.000 | 27.35 |
| ATOM | 3765 | CE1 | PHE | B | 187 | 45.074 | 39.304 | 73.230 | 1.000 | 20.96 |
| ATOM | 3766 | CZ  | PHE | B | 187 | 45.244 | 39.654 | 74.558 | 1.000 | 27.74 |
| ATOM | 3767 | CE2 | PHE | B | 187 | 45.589 | 40.951 | 74.882 | 1.000 | 33.31 |
| ATOM | 3768 | CD2 | PHE | B | 187 | 45.760 | 41.891 | 73.884 | 1.000 | 33.33 |
| ATOM | 3769 | C   | PHE | B | 187 | 44.937 | 44.474 | 70.079 | 1.000 | 32.36 |
| ATOM | 3770 | O   | PHE | B | 187 | 44.466 | 44.149 | 68.989 | 1.000 | 24.82 |
| ATOM | 3771 | N   | LYS | B | 188 | 45.731 | 45.502 | 70.304 | 1.000 | 33.51 |
| ATOM | 3772 | CA  | LYS | B | 188 | 46.366 | 46.294 | 69.265 | 1.000 | 39.34 |
| ATOM | 3773 | CB  | LYS | B | 188 | 46.107 | 47.786 | 69.445 | 1.000 | 52.27 |
| ATOM | 3774 | CG  | LYS | B | 188 | 47.360 | 48.631 | 69.623 | 1.000 | 65.67 |
| ATOM | 3775 | CD  | LYS | B | 188 | 47.208 | 49.980 | 68.916 | 1.000 | 71.88 |
| ATOM | 3776 | CE  | LYS | B | 188 | 48.299 | 50.947 | 69.345 | 1.000 | 76.68 |
| ATOM | 3777 | NZ  | LYS | B | 188 | 48.492 | 52.055 | 68.375 | 1.000 | 77.91 |
| ATOM | 3778 | C   | LYS | B | 188 | 47.867 | 46.005 | 69.285 | 1.000 | 31.64 |
| ATOM | 3779 | O   | LYS | B | 188 | 48.496 | 46.016 | 70.345 | 1.000 | 31.25 |
| ATOM | 3780 | N   | ILE | B | 189 | 48.432 | 45.740 | 68.110 | 1.000 | 25.97 |
| ATOM | 3781 | CA  | ILE | B | 189 | 49.869 | 45.521 | 68.045 | 1.000 | 32.80 |
| ATOM | 3782 | CB  | ILE | B | 189 | 50.247 | 44.098 | 67.612 | 1.000 | 38.71 |
| ATOM | 3783 | CG1 | ILE | B | 189 | 49.093 | 43.327 | 66.974 | 1.000 | 46.51 |
| ATOM | 3784 | CD1 | ILE | B | 189 | 48.715 | 43.822 | 65.594 | 1.000 | 39.76 |
| ATOM | 3785 | CG2 | ILE | B | 189 | 50.838 | 43.337 | 68.787 | 1.000 | 53.93 |
| ATOM | 3786 | C   | ILE | B | 189 | 50.485 | 46.515 | 67.066 | 1.000 | 33.72 |
| ATOM | 3787 | O   | ILE | B | 189 | 49.888 | 46.777 | 66.022 | 1.000 | 37.58 |
| ATOM | 3788 | N   | CYS | B | 190 | 51.648 | 47.022 | 67.450 | 1.000 | 30.23 |
| ATOM | 3789 | CA  | CYS | B | 190 | 52.400 | 47.934 | 66.602 | 1.000 | 40.89 |
| ATOM | 3790 | CB  | CYS | B | 190 | 52.596 | 49.307 | 67.233 | 1.000 | 42.64 |
| ATOM | 3791 | SG  | CYS | B | 190 | 51.150 | 50.118 | 67.926 | 1.000 | 58.03 |
| ATOM | 3792 | C   | CYS | B | 190 | 53.775 | 47.334 | 66.282 | 1.000 | 44.57 |
| ATOM | 3793 | O   | CYS | B | 190 | 54.446 | 46.804 | 67.173 | 1.000 | 40.52 |
| ATOM | 3794 | N   | GLY | B | 191 | 54.140 | 47.444 | 65.011 | 1.000 | 36.59 |
| ATOM | 3795 | CA  | GLY | B | 191 | 55.407 | 46.950 | 64.504 | 1.000 | 43.85 |

**FIGURE 79**

|      |      |     |     |   |     |        |        |        |       |        |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|--------|
| ATOM | 3796 | C   | GLY | B | 191 | 56.063 | 48.026 | 63.654 | 1.000 | 51.14  |
| ATOM | 3797 | O   | GLY | B | 191 | 55.515 | 49.122 | 63.561 | 1.000 | 44.72  |
| ATOM | 3798 | N   | GLU | B | 192 | 57.206 | 47.732 | 63.051 | 1.000 | 65.39  |
| ATOM | 3799 | CA  | GLU | B | 192 | 57.917 | 48.729 | 62.251 | 1.000 | 74.92  |
| ATOM | 3800 | CB  | GLU | B | 192 | 59.164 | 48.118 | 61.620 | 1.000 | 80.08  |
| ATOM | 3801 | CG  | GLU | B | 192 | 59.486 | 46.705 | 62.068 | 1.000 | 89.69  |
| ATOM | 3802 | CD  | GLU | B | 192 | 60.187 | 46.619 | 63.406 | 1.000 | 99.45  |
| ATOM | 3803 | OE1 | GLU | B | 192 | 59.909 | 45.653 | 64.155 | 1.000 | 109.46 |
| ATOM | 3804 | OE2 | GLU | B | 192 | 61.017 | 47.500 | 63.734 | 1.000 | 105.75 |
| ATOM | 3805 | C   | GLU | B | 192 | 56.982 | 49.325 | 61.190 | 1.000 | 77.53  |
| ATOM | 3806 | O   | GLU | B | 192 | 57.093 | 50.520 | 60.921 | 1.000 | 71.90  |
| ATOM | 3807 | N   | GLU | B | 193 | 56.119 | 48.468 | 60.689 | 1.000 | 80.23  |
| ATOM | 3808 | CA  | GLU | B | 193 | 55.037 | 48.642 | 59.748 | 1.000 | 85.66  |
| ATOM | 3809 | CB  | GLU | B | 193 | 54.717 | 50.116 | 59.508 | 1.000 | 94.37  |
| ATOM | 3810 | CG  | GLU | B | 193 | 53.928 | 50.436 | 58.253 | 1.000 | 106.40 |
| ATOM | 3811 | CD  | GLU | B | 193 | 52.595 | 49.734 | 58.174 | 1.000 | 115.65 |
| ATOM | 3812 | OE1 | GLU | B | 193 | 51.537 | 50.403 | 58.158 | 1.000 | 130.32 |
| ATOM | 3813 | OE2 | GLU | B | 193 | 52.613 | 48.478 | 58.138 | 1.000 | 120.48 |
| ATOM | 3814 | C   | GLU | B | 193 | 55.364 | 47.949 | 58.424 | 1.000 | 90.24  |
| ATOM | 3815 | O   | GLU | B | 193 | 56.248 | 48.389 | 57.684 | 1.000 | 99.18  |
| ATOM | 3816 | N   | GLN | B | 194 | 54.652 | 46.858 | 58.146 | 1.000 | 94.55  |
| ATOM | 3817 | CA  | GLN | B | 194 | 54.801 | 46.130 | 56.892 | 1.000 | 99.07  |
| ATOM | 3818 | CB  | GLN | B | 194 | 55.799 | 44.984 | 57.030 | 1.000 | 99.47  |
| ATOM | 3819 | CG  | GLN | B | 194 | 56.655 | 45.014 | 58.284 | 1.000 | 99.46  |
| ATOM | 3820 | CD  | GLN | B | 194 | 58.097 | 44.616 | 58.010 | 1.000 | 96.93  |
| ATOM | 3821 | OE1 | GLN | B | 194 | 58.678 | 44.953 | 56.977 | 1.000 | 92.58  |
| ATOM | 3822 | NE2 | GLN | B | 194 | 58.682 | 43.863 | 58.944 | 1.000 | 90.47  |
| ATOM | 3823 | C   | GLN | B | 194 | 53.449 | 45.595 | 56.413 | 1.000 | 102.41 |
| ATOM | 3824 | O   | GLN | B | 194 | 53.158 | 44.410 | 56.574 | 1.000 | 106.43 |
| ATOM | 3825 | N   | LEU | B | 195 | 52.649 | 46.481 | 55.833 | 1.000 | 102.43 |
| ATOM | 3826 | CA  | LEU | B | 195 | 51.322 | 46.214 | 55.301 | 1.000 | 100.78 |
| ATOM | 3827 | CB  | LEU | B | 195 | 51.291 | 44.888 | 54.539 | 1.000 | 96.19  |
| ATOM | 3828 | CG  | LEU | B | 195 | 51.096 | 44.962 | 53.021 | 1.000 | 88.64  |
| ATOM | 3829 | CD1 | LEU | B | 195 | 51.473 | 46.333 | 52.484 | 1.000 | 68.61  |
| ATOM | 3830 | CD2 | LEU | B | 195 | 51.917 | 43.868 | 52.320 | 1.000 | 77.73  |
| ATOM | 3831 | C   | LEU | B | 195 | 50.270 | 46.236 | 56.412 | 1.000 | 101.84 |
| ATOM | 3832 | O   | LEU | B | 195 | 49.132 | 45.812 | 56.210 | 1.000 | 107.43 |
| ATOM | 3833 | N   | ASP | B | 196 | 50.667 | 46.740 | 57.570 | 1.000 | 100.14 |
| ATOM | 3834 | CA  | ASP | B | 196 | 49.834 | 46.918 | 58.754 | 1.000 | 95.50  |
| ATOM | 3835 | CB  | ASP | B | 196 | 49.258 | 45.605 | 59.253 | 1.000 | 93.87  |
| ATOM | 3836 | CG  | ASP | B | 196 | 50.159 | 44.699 | 60.049 | 1.000 | 86.73  |
| ATOM | 3837 | OD1 | ASP | B | 196 | 51.251 | 44.300 | 59.589 | 1.000 | 56.18  |
| ATOM | 3838 | OD2 | ASP | B | 196 | 49.770 | 44.325 | 61.183 | 1.000 | 68.86  |
| ATOM | 3839 | C   | ASP | B | 196 | 50.665 | 47.613 | 59.833 | 1.000 | 91.65  |
| ATOM | 3840 | O   | ASP | B | 196 | 51.757 | 47.144 | 60.157 | 1.000 | 97.39  |
| ATOM | 3841 | N   | ALA | B | 197 | 50.175 | 48.732 | 60.358 | 1.000 | 87.23  |
| ATOM | 3842 | CA  | ALA | B | 197 | 50.971 | 49.522 | 61.291 | 1.000 | 84.73  |
| ATOM | 3843 | CB  | ALA | B | 197 | 51.043 | 50.971 | 60.832 | 1.000 | 82.95  |
| ATOM | 3844 | C   | ALA | B | 197 | 50.426 | 49.456 | 62.716 | 1.000 | 82.50  |
| ATOM | 3845 | O   | ALA | B | 197 | 51.192 | 49.650 | 63.662 | 1.000 | 66.61  |
| ATOM | 3846 | N   | HIS | B | 198 | 49.132 | 49.213 | 62.833 | 1.000 | 82.67  |
| ATOM | 3847 | CA  | HIS | B | 198 | 48.373 | 49.029 | 64.057 | 1.000 | 77.93  |

**FIGURE 80**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3848 | CB  | HIS | B | 198 | 47.927 | 50.338 | 64.697 | 1.000 | 77.67 |
| ATOM | 3849 | CG  | HIS | B | 198 | 48.200 | 51.573 | 63.899 | 1.000 | 84.79 |
| ATOM | 3850 | ND1 | HIS | B | 198 | 47.669 | 51.785 | 62.645 | 1.000 | 86.88 |
| ATOM | 3851 | CE1 | HIS | B | 198 | 48.085 | 52.952 | 62.182 | 1.000 | 88.81 |
| ATOM | 3852 | NE2 | HIS | B | 198 | 48.869 | 53.503 | 63.089 | 1.000 | 87.71 |
| ATOM | 3853 | CD2 | HIS | B | 198 | 48.959 | 52.659 | 64.170 | 1.000 | 85.49 |
| ATOM | 3854 | C   | HIS | B | 198 | 47.141 | 48.164 | 63.752 | 1.000 | 75.55 |
| ATOM | 3855 | O   | HIS | B | 198 | 46.055 | 48.678 | 63.493 | 1.000 | 83.33 |
| ATOM | 3856 | N   | ARG | B | 199 | 47.365 | 46.860 | 63.783 | 1.000 | 63.26 |
| ATOM | 3857 | CA  | ARG | B | 199 | 46.380 | 45.839 | 63.475 | 1.000 | 55.42 |
| ATOM | 3858 | CB  | ARG | B | 199 | 47.074 | 44.642 | 62.808 | 1.000 | 56.72 |
| ATOM | 3859 | CG  | ARG | B | 199 | 46.181 | 43.423 | 62.663 | 1.000 | 47.99 |
| ATOM | 3860 | CD  | ARG | B | 199 | 46.961 | 42.174 | 62.308 | 1.000 | 37.39 |
| ATOM | 3861 | NE  | ARG | B | 199 | 48.216 | 42.423 | 61.614 | 1.000 | 35.84 |
| ATOM | 3862 | CZ  | ARG | B | 199 | 49.253 | 41.591 | 61.677 | 1.000 | 43.79 |
| ATOM | 3863 | NH1 | ARG | B | 199 | 49.171 | 40.475 | 62.398 | 1.000 | 20.33 |
| ATOM | 3864 | NH2 | ARG | B | 199 | 50.368 | 41.875 | 61.018 | 1.000 | 25.11 |
| ATOM | 3865 | C   | ARG | B | 199 | 45.629 | 45.376 | 64.717 | 1.000 | 43.83 |
| ATOM | 3866 | O   | ARG | B | 199 | 46.181 | 45.353 | 65.817 | 1.000 | 40.98 |
| ATOM | 3867 | N   | LEU | B | 200 | 44.361 | 45.010 | 64.551 | 1.000 | 35.65 |
| ATOM | 3868 | CA  | LEU | B | 200 | 43.571 | 44.511 | 65.672 | 1.000 | 34.82 |
| ATOM | 3869 | CB  | LEU | B | 200 | 42.096 | 44.866 | 65.560 | 1.000 | 37.89 |
| ATOM | 3870 | CG  | LEU | B | 200 | 41.296 | 45.146 | 66.831 | 1.000 | 47.74 |
| ATOM | 3871 | CD1 | LEU | B | 200 | 41.329 | 43.974 | 67.800 | 1.000 | 44.43 |
| ATOM | 3872 | CD2 | LEU | B | 200 | 41.794 | 46.411 | 67.514 | 1.000 | 55.08 |
| ATOM | 3873 | C   | LEU | B | 200 | 43.707 | 42.991 | 65.738 | 1.000 | 36.55 |
| ATOM | 3874 | O   | LEU | B | 200 | 43.563 | 42.331 | 64.706 | 1.000 | 39.15 |
| ATOM | 3875 | N   | ILE | B | 201 | 43.977 | 42.484 | 66.938 | 1.000 | 29.95 |
| ATOM | 3876 | CA  | ILE | B | 201 | 44.033 | 41.033 | 67.101 | 1.000 | 25.47 |
| ATOM | 3877 | CB  | ILE | B | 201 | 45.314 | 40.531 | 67.770 | 1.000 | 25.78 |
| ATOM | 3878 | CG1 | ILE | B | 201 | 46.630 | 40.929 | 67.102 | 1.000 | 24.11 |
| ATOM | 3879 | CD1 | ILE | B | 201 | 46.743 | 40.486 | 65.660 | 1.000 | 22.88 |
| ATOM | 3880 | CG2 | ILE | B | 201 | 45.271 | 39.009 | 67.912 | 1.000 | 28.86 |
| ATOM | 3881 | C   | ILE | B | 201 | 42.824 | 40.609 | 67.935 | 1.000 | 25.30 |
| ATOM | 3882 | O   | ILE | B | 201 | 42.468 | 41.326 | 68.864 | 1.000 | 36.64 |
| ATOM | 3883 | N   | ARG | B | 202 | 42.229 | 39.478 | 67.597 | 1.000 | 29.04 |
| ATOM | 3884 | CA  | ARG | B | 202 | 41.111 | 38.919 | 68.353 | 1.000 | 28.15 |
| ATOM | 3885 | CB  | ARG | B | 202 | 39.928 | 38.698 | 67.421 | 1.000 | 32.44 |
| ATOM | 3886 | CG  | ARG | B | 202 | 38.587 | 39.177 | 67.941 | 1.000 | 38.49 |
| ATOM | 3887 | CD  | ARG | B | 202 | 38.061 | 40.347 | 67.121 | 1.000 | 51.50 |
| ATOM | 3888 | NE  | ARG | B | 202 | 36.996 | 41.057 | 67.815 | 1.000 | 62.80 |
| ATOM | 3889 | CZ  | ARG | B | 202 | 36.709 | 42.345 | 67.754 | 1.000 | 72.90 |
| ATOM | 3890 | NH1 | ARG | B | 202 | 37.410 | 43.184 | 67.004 | 1.000 | 64.58 |
| ATOM | 3891 | NH2 | ARG | B | 202 | 35.690 | 42.818 | 68.467 | 1.000 | 95.35 |
| ATOM | 3892 | C   | ARG | B | 202 | 41.552 | 37.621 | 69.013 | 1.000 | 24.66 |
| ATOM | 3893 | O   | ARG | B | 202 | 41.976 | 36.706 | 68.299 | 1.000 | 31.26 |
| ATOM | 3894 | N   | HIS | B | 203 | 41.479 | 37.532 | 70.330 | 1.000 | 19.54 |
| ATOM | 3895 | CA  | HIS | B | 203 | 41.943 | 36.336 | 71.046 | 1.000 | 27.13 |
| ATOM | 3896 | CB  | HIS | B | 203 | 43.011 | 36.754 | 72.047 | 1.000 | 23.50 |
| ATOM | 3897 | CG  | HIS | B | 203 | 43.762 | 35.711 | 72.798 | 1.000 | 26.59 |
| ATOM | 3898 | ND1 | HIS | B | 203 | 43.264 | 35.062 | 73.902 | 1.000 | 33.06 |
| ATOM | 3899 | CE1 | HIS | B | 203 | 44.154 | 34.200 | 74.365 | 1.000 | 29.95 |

**FIGURE 81**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3900 | NE2 | HIS | B | 203 | 45.231 | 34.264 | 73.603 | 1.000 | 28.32 |
| ATOM | 3901 | CD2 | HIS | B | 203 | 45.012 | 35.203 | 72.620 | 1.000 | 29.08 |
| ATOM | 3902 | C   | HIS | B | 203 | 40.790 | 35.608 | 71.729 | 1.000 | 29.92 |
| ATOM | 3903 | O   | HIS | B | 203 | 40.060 | 36.152 | 72.557 | 1.000 | 25.16 |
| ATOM | 3904 | N   | PHE | B | 204 | 40.599 | 34.337 | 71.385 | 1.000 | 23.26 |
| ATOM | 3905 | CA  | PHE | B | 204 | 39.474 | 33.561 | 71.878 | 1.000 | 17.30 |
| ATOM | 3906 | CB  | PHE | B | 204 | 38.735 | 32.923 | 70.702 | 1.000 | 21.59 |
| ATOM | 3907 | CG  | PHE | B | 204 | 38.310 | 33.929 | 69.657 | 1.000 | 29.41 |
| ATOM | 3908 | CD1 | PHE | B | 204 | 39.097 | 34.183 | 68.548 | 1.000 | 28.21 |
| ATOM | 3909 | CE1 | PHE | B | 204 | 38.720 | 35.091 | 67.585 | 1.000 | 29.05 |
| ATOM | 3910 | CZ  | PHE | B | 204 | 37.537 | 35.792 | 67.732 | 1.000 | 29.20 |
| ATOM | 3911 | CE2 | PHE | B | 204 | 36.737 | 35.544 | 68.829 | 1.000 | 29.69 |
| ATOM | 3912 | CD2 | PHE | B | 204 | 37.114 | 34.616 | 69.779 | 1.000 | 29.48 |
| ATOM | 3913 | C   | PHE | B | 204 | 39.947 | 32.481 | 72.844 | 1.000 | 28.09 |
| ATOM | 3914 | O   | PHE | B | 204 | 40.557 | 31.502 | 72.406 | 1.000 | 31.26 |
| ATOM | 3915 | N   | HIS | B | 205 | 39.676 | 32.681 | 74.133 | 1.000 | 18.80 |
| ATOM | 3916 | CA  | HIS | B | 205 | 40.188 | 31.784 | 75.156 | 1.000 | 21.65 |
| ATOM | 3917 | CB  | HIS | B | 205 | 40.883 | 32.621 | 76.249 | 1.000 | 23.81 |
| ATOM | 3918 | CG  | HIS | B | 205 | 41.692 | 31.816 | 77.216 | 1.000 | 24.84 |
| ATOM | 3919 | ND1 | HIS | B | 205 | 42.280 | 32.371 | 78.328 | 1.000 | 29.84 |
| ATOM | 3920 | CE1 | HIS | B | 205 | 42.931 | 31.440 | 78.997 | 1.000 | 32.02 |
| ATOM | 3921 | NE2 | HIS | B | 205 | 42.793 | 30.285 | 78.364 | 1.000 | 25.82 |
| ATOM | 3922 | CD2 | HIS | B | 205 | 42.029 | 30.502 | 77.251 | 1.000 | 28.58 |
| ATOM | 3923 | C   | HIS | B | 205 | 39.114 | 30.895 | 75.778 | 1.000 | 28.42 |
| ATOM | 3924 | O   | HIS | B | 205 | 38.277 | 31.351 | 76.564 | 1.000 | 24.92 |
| ATOM | 3925 | N   | TYR | B | 206 | 39.190 | 29.613 | 75.438 | 1.000 | 26.78 |
| ATOM | 3926 | CA  | TYR | B | 206 | 38.347 | 28.572 | 76.005 | 1.000 | 25.27 |
| ATOM | 3927 | CB  | TYR | B | 206 | 38.308 | 27.361 | 75.091 | 1.000 | 25.32 |
| ATOM | 3928 | CG  | TYR | B | 206 | 37.302 | 26.289 | 75.429 | 1.000 | 21.60 |
| ATOM | 3929 | CD1 | TYR | B | 206 | 35.946 | 26.502 | 75.229 | 1.000 | 21.30 |
| ATOM | 3930 | CE1 | TYR | B | 206 | 35.027 | 25.519 | 75.537 | 1.000 | 22.97 |
| ATOM | 3931 | CZ  | TYR | B | 206 | 35.457 | 24.313 | 76.039 | 1.000 | 26.67 |
| ATOM | 3932 | OH  | TYR | B | 206 | 34.536 | 23.336 | 76.341 | 1.000 | 53.16 |
| ATOM | 3933 | CE2 | TYR | B | 206 | 36.799 | 24.073 | 76.248 | 1.000 | 25.66 |
| ATOM | 3934 | CD2 | TYR | B | 206 | 37.708 | 25.067 | 75.939 | 1.000 | 23.88 |
| ATOM | 3935 | C   | TYR | B | 206 | 38.850 | 28.115 | 77.369 | 1.000 | 23.63 |
| ATOM | 3936 | O   | TYR | B | 206 | 39.927 | 27.531 | 77.442 | 1.000 | 22.75 |
| ATOM | 3937 | N   | THR | B | 207 | 38.078 | 28.362 | 78.419 | 1.000 | 28.47 |
| ATOM | 3938 | CA  | THR | B | 207 | 38.594 | 28.239 | 79.781 | 1.000 | 34.58 |
| ATOM | 3939 | CB  | THR | B | 207 | 38.251 | 29.523 | 80.579 | 1.000 | 29.68 |
| ATOM | 3940 | OG1 | THR | B | 207 | 36.868 | 29.844 | 80.409 | 1.000 | 32.12 |
| ATOM | 3941 | CG2 | THR | B | 207 | 39.025 | 30.717 | 80.039 | 1.000 | 27.42 |
| ATOM | 3942 | C   | THR | B | 207 | 38.079 | 27.031 | 80.540 | 1.000 | 38.19 |
| ATOM | 3943 | O   | THR | B | 207 | 38.351 | 26.891 | 81.740 | 1.000 | 46.50 |
| ATOM | 3944 | N   | VAL | B | 208 | 37.333 | 26.118 | 79.912 | 1.000 | 36.23 |
| ATOM | 3945 | CA  | VAL | B | 208 | 36.752 | 25.066 | 80.760 | 1.000 | 32.80 |
| ATOM | 3946 | CB  | VAL | B | 208 | 35.226 | 25.275 | 80.831 | 1.000 | 28.19 |
| ATOM | 3947 | CG1 | VAL | B | 208 | 34.942 | 26.537 | 81.638 | 1.000 | 27.38 |
| ATOM | 3948 | CG2 | VAL | B | 208 | 34.601 | 25.387 | 79.454 | 1.000 | 32.82 |
| ATOM | 3949 | C   | VAL | B | 208 | 37.089 | 23.660 | 80.314 | 1.000 | 39.69 |
| ATOM | 3950 | O   | VAL | B | 208 | 36.491 | 22.707 | 80.825 | 1.000 | 41.93 |
| ATOM | 3951 | N   | TRP | B | 209 | 38.039 | 23.467 | 79.397 | 1.000 | 40.70 |

FIGURE 82

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 3952 | CA  | TRP | B | 209 | 38.445 | 22.102 | 79.049 | 1.000 | 36.47 |
| ATOM | 3953 | CB  | TRP | B | 209 | 39.577 | 22.083 | 78.032 | 1.000 | 31.02 |
| ATOM | 3954 | CG  | TRP | B | 209 | 39.652 | 20.846 | 77.194 | 1.000 | 28.16 |
| ATOM | 3955 | CD1 | TRP | B | 209 | 39.949 | 19.583 | 77.597 | 1.000 | 27.98 |
| ATOM | 3956 | NE1 | TRP | B | 209 | 39.921 | 18.716 | 76.527 | 1.000 | 33.60 |
| ATOM | 3957 | CE2 | TRP | B | 209 | 39.600 | 19.427 | 75.396 | 1.000 | 27.75 |
| ATOM | 3958 | CD2 | TRP | B | 209 | 39.426 | 20.768 | 75.775 | 1.000 | 24.17 |
| ATOM | 3959 | CE3 | TRP | B | 209 | 39.092 | 21.719 | 74.805 | 1.000 | 28.32 |
| ATOM | 3960 | CZ3 | TRP | B | 209 | 38.941 | 21.300 | 73.496 | 1.000 | 34.71 |
| ATOM | 3961 | CH2 | TRP | B | 209 | 39.121 | 19.954 | 73.151 | 1.000 | 31.19 |
| ATOM | 3962 | CZ2 | TRP | B | 209 | 39.450 | 18.999 | 74.078 | 1.000 | 21.94 |
| ATOM | 3963 | C   | TRP | B | 209 | 38.888 | 21.358 | 80.309 | 1.000 | 39.28 |
| ATOM | 3964 | O   | TRP | B | 209 | 39.737 | 21.872 | 81.039 | 1.000 | 33.04 |
| ATOM | 3965 | N   | PRO | B | 210 | 38.325 | 20.185 | 80.563 | 1.000 | 38.49 |
| ATOM | 3966 | CA  | PRO | B | 210 | 38.574 | 19.480 | 81.825 | 1.000 | 33.55 |
| ATOM | 3967 | CB  | PRO | B | 210 | 37.657 | 18.251 | 81.742 | 1.000 | 33.67 |
| ATOM | 3968 | CG  | PRO | B | 210 | 36.654 | 18.591 | 80.688 | 1.000 | 33.65 |
| ATOM | 3969 | CD  | PRO | B | 210 | 37.408 | 19.429 | 79.689 | 1.000 | 31.99 |
| ATOM | 3970 | C   | PRO | B | 210 | 40.020 | 19.024 | 81.943 | 1.000 | 39.20 |
| ATOM | 3971 | O   | PRO | B | 210 | 40.737 | 18.955 | 80.943 | 1.000 | 45.02 |
| ATOM | 3972 | N   | ASP | B | 211 | 40.425 | 18.710 | 83.167 | 1.000 | 42.94 |
| ATOM | 3973 | CA  | ASP | B | 211 | 41.772 | 18.214 | 83.426 | 1.000 | 48.87 |
| ATOM | 3974 | CB  | ASP | B | 211 | 42.010 | 18.080 | 84.934 | 1.000 | 57.39 |
| ATOM | 3975 | CG  | ASP | B | 211 | 42.375 | 19.402 | 85.586 | 1.000 | 66.45 |
| ATOM | 3976 | OD1 | ASP | B | 211 | 42.136 | 20.463 | 84.966 | 1.000 | 52.25 |
| ATOM | 3977 | OD2 | ASP | B | 211 | 42.903 | 19.369 | 86.721 | 1.000 | 87.29 |
| ATOM | 3978 | C   | ASP | B | 211 | 42.020 | 16.872 | 82.747 | 1.000 | 39.83 |
| ATOM | 3979 | O   | ASP | B | 211 | 43.122 | 16.559 | 82.300 | 1.000 | 47.17 |
| ATOM | 3980 | N   | HIS | B | 212 | 40.987 | 16.044 | 82.672 | 1.000 | 40.86 |
| ATOM | 3981 | CA  | HIS | B | 212 | 41.117 | 14.730 | 82.050 | 1.000 | 47.36 |
| ATOM | 3982 | CB  | HIS | B | 212 | 41.076 | 13.599 | 83.066 | 1.000 | 59.57 |
| ATOM | 3983 | CG  | HIS | B | 212 | 42.146 | 13.536 | 84.102 | 1.000 | 71.70 |
| ATOM | 3984 | ND1 | HIS | B | 212 | 42.060 | 14.183 | 85.313 | 1.000 | 74.03 |
| ATOM | 3985 | CE1 | HIS | B | 212 | 43.144 | 13.953 | 86.032 | 1.000 | 77.44 |
| ATOM | 3986 | NE2 | HIS | B | 212 | 43.938 | 13.155 | 85.336 | 1.000 | 79.18 |
| ATOM | 3987 | CD2 | HIS | B | 212 | 43.332 | 12.879 | 84.131 | 1.000 | 78.65 |
| ATOM | 3988 | C   | HIS | B | 212 | 39.976 | 14.556 | 81.049 | 1.000 | 44.25 |
| ATOM | 3989 | O   | HIS | B | 212 | 38.865 | 14.996 | 81.354 | 1.000 | 50.41 |
| ATOM | 3990 | N   | GLY | B | 213 | 40.237 | 13.936 | 79.906 | 1.000 | 43.28 |
| ATOM | 3991 | CA  | GLY | B | 213 | 39.210 | 13.707 | 78.905 | 1.000 | 34.05 |
| ATOM | 3992 | C   | GLY | B | 213 | 38.716 | 14.968 | 78.223 | 1.000 | 36.21 |
| ATOM | 3993 | O   | GLY | B | 213 | 39.361 | 16.015 | 78.258 | 1.000 | 46.36 |
| ATOM | 3994 | N   | VAL | B | 214 | 37.550 | 14.875 | 77.595 | 1.000 | 38.56 |
| ATOM | 3995 | CA  | VAL | B | 214 | 36.931 | 15.933 | 76.818 | 1.000 | 39.41 |
| ATOM | 3996 | CB  | VAL | B | 214 | 36.356 | 15.345 | 75.510 | 1.000 | 40.18 |
| ATOM | 3997 | CG1 | VAL | B | 214 | 37.467 | 14.671 | 74.725 | 1.000 | 35.68 |
| ATOM | 3998 | CG2 | VAL | B | 214 | 35.226 | 14.382 | 75.831 | 1.000 | 48.90 |
| ATOM | 3999 | C   | VAL | B | 214 | 35.809 | 16.620 | 77.575 | 1.000 | 43.12 |
| ATOM | 4000 | O   | VAL | B | 214 | 35.366 | 16.105 | 78.602 | 1.000 | 64.15 |
| ATOM | 4001 | N   | PRO | B | 215 | 35.344 | 17.763 | 77.089 | 1.000 | 42.93 |
| ATOM | 4002 | CA  | PRO | B | 215 | 34.151 | 18.378 | 77.679 | 1.000 | 40.14 |
| ATOM | 4003 | CB  | PRO | B | 215 | 33.784 | 19.448 | 76.653 | 1.000 | 42.40 |

**FIGURE 83**

|      |      |     |           |        |        |        |       |       |
|------|------|-----|-----------|--------|--------|--------|-------|-------|
| ATOM | 4004 | CG  | PRO B 215 | 35.090 | 19.835 | 76.040 | 1.000 | 41.27 |
| ATOM | 4005 | CD  | PRO B 215 | 35.888 | 18.567 | 75.982 | 1.000 | 37.96 |
| ATOM | 4006 | C   | PRO B 215 | 33.008 | 17.374 | 77.800 | 1.000 | 45.59 |
| ATOM | 4007 | O   | PRO B 215 | 32.766 | 16.617 | 76.859 | 1.000 | 40.94 |
| ATOM | 4008 | N   | GLU B 216 | 32.333 | 17.381 | 78.942 | 1.000 | 50.95 |
| ATOM | 4009 | CA  | GLU B 216 | 31.204 | 16.498 | 79.215 | 1.000 | 53.03 |
| ATOM | 4010 | CB  | GLU B 216 | 30.693 | 16.699 | 80.643 | 1.000 | 59.73 |
| ATOM | 4011 | CG  | GLU B 216 | 29.489 | 15.856 | 81.030 | 1.000 | 65.18 |
| ATOM | 4012 | CD  | GLU B 216 | 28.745 | 16.402 | 82.236 | 1.000 | 71.96 |
| ATOM | 4013 | OE1 | GLU B 216 | 29.388 | 16.616 | 83.292 | 1.000 | 79.59 |
| ATOM | 4014 | OE2 | GLU B 216 | 27.515 | 16.622 | 82.138 | 1.000 | 56.48 |
| ATOM | 4015 | C   | GLU B 216 | 30.083 | 16.748 | 78.217 | 1.000 | 50.99 |
| ATOM | 4016 | O   | GLU B 216 | 29.274 | 15.873 | 77.907 | 1.000 | 49.11 |
| ATOM | 4017 | N   | THR B 217 | 30.038 | 17.981 | 77.699 | 1.000 | 46.20 |
| ATOM | 4018 | CA  | THR B 217 | 29.017 | 18.266 | 76.693 | 1.000 | 46.03 |
| ATOM | 4019 | CB  | THR B 217 | 28.092 | 19.430 | 77.079 | 1.000 | 38.73 |
| ATOM | 4020 | OG1 | THR B 217 | 26.778 | 19.154 | 76.564 | 1.000 | 61.70 |
| ATOM | 4021 | CG2 | THR B 217 | 28.539 | 20.738 | 76.440 | 1.000 | 30.35 |
| ATOM | 4022 | C   | THR B 217 | 29.666 | 18.582 | 75.347 | 1.000 | 49.34 |
| ATOM | 4023 | O   | THR B 217 | 30.797 | 19.060 | 75.290 | 1.000 | 48.39 |
| ATOM | 4024 | N   | THR B 218 | 28.918 | 18.307 | 74.287 | 1.000 | 45.15 |
| ATOM | 4025 | CA  | THR B 218 | 29.328 | 18.657 | 72.938 | 1.000 | 38.83 |
| ATOM | 4026 | CB  | THR B 218 | 28.599 | 17.780 | 71.908 | 1.000 | 40.05 |
| ATOM | 4027 | OG1 | THR B 218 | 27.195 | 18.052 | 72.006 | 1.000 | 47.92 |
| ATOM | 4028 | CG2 | THR B 218 | 28.789 | 16.302 | 72.204 | 1.000 | 37.44 |
| ATOM | 4029 | C   | THR B 218 | 29.025 | 20.122 | 72.648 | 1.000 | 40.85 |
| ATOM | 4030 | O   | THR B 218 | 29.781 | 20.830 | 71.985 | 1.000 | 49.43 |
| ATOM | 4031 | N   | GLN B 219 | 27.886 | 20.590 | 73.149 | 1.000 | 39.19 |
| ATOM | 4032 | CA  | GLN B 219 | 27.423 | 21.943 | 72.863 | 1.000 | 40.36 |
| ATOM | 4033 | CB  | GLN B 219 | 26.112 | 22.238 | 73.599 | 1.000 | 47.97 |
| ATOM | 4034 | CG  | GLN B 219 | 25.063 | 22.954 | 72.773 | 1.000 | 57.22 |
| ATOM | 4035 | CD  | GLN B 219 | 24.636 | 24.294 | 73.334 | 1.000 | 65.42 |
| ATOM | 4036 | OE1 | GLN B 219 | 24.948 | 24.653 | 74.471 | 1.000 | 76.84 |
| ATOM | 4037 | NE2 | GLN B 219 | 23.901 | 25.061 | 72.531 | 1.000 | 73.40 |
| ATOM | 4038 | C   | GLN B 219 | 28.486 | 22.976 | 73.229 | 1.000 | 40.36 |
| ATOM | 4039 | O   | GLN B 219 | 28.610 | 23.987 | 72.535 | 1.000 | 40.22 |
| ATOM | 4040 | N   | SER B 220 | 29.229 | 22.716 | 74.293 | 1.000 | 38.53 |
| ATOM | 4041 | CA  | SER B 220 | 30.296 | 23.588 | 74.774 | 1.000 | 40.28 |
| ATOM | 4042 | CB  | SER B 220 | 31.039 | 22.897 | 75.927 | 1.000 | 36.16 |
| ATOM | 4043 | OG  | SER B 220 | 31.787 | 23.830 | 76.681 | 1.000 | 43.68 |
| ATOM | 4044 | C   | SER B 220 | 31.282 | 23.969 | 73.678 | 1.000 | 39.40 |
| ATOM | 4045 | O   | SER B 220 | 31.451 | 25.138 | 73.322 | 1.000 | 40.25 |
| ATOM | 4046 | N   | LEU B 221 | 31.977 | 22.990 | 73.102 | 1.000 | 42.59 |
| ATOM | 4047 | CA  | LEU B 221 | 32.991 | 23.314 | 72.093 | 1.000 | 37.94 |
| ATOM | 4048 | CB  | LEU B 221 | 33.912 | 22.118 | 71.864 | 1.000 | 36.81 |
| ATOM | 4049 | CG  | LEU B 221 | 35.282 | 22.419 | 71.247 | 1.000 | 44.42 |
| ATOM | 4050 | CD1 | LEU B 221 | 36.044 | 23.445 | 72.073 | 1.000 | 31.31 |
| ATOM | 4051 | CD2 | LEU B 221 | 36.111 | 21.152 | 71.101 | 1.000 | 39.34 |
| ATOM | 4052 | C   | LEU B 221 | 32.323 | 23.778 | 70.805 | 1.000 | 37.27 |
| ATOM | 4053 | O   | LEU B 221 | 32.776 | 24.708 | 70.136 | 1.000 | 50.72 |
| ATOM | 4054 | N   | ILE B 222 | 31.217 | 23.135 | 70.456 | 1.000 | 35.78 |
| ATOM | 4055 | CA  | ILE B 222 | 30.451 | 23.526 | 69.277 | 1.000 | 40.80 |

**FIGURE 84**



Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4056 | CB  | ILE | B | 222 | 29.169 | 22.678 | 69.172 | 1.000 | 36.72 |
| ATOM | 4057 | CG1 | ILE | B | 222 | 29.431 | 21.240 | 68.707 | 1.000 | 28.35 |
| ATOM | 4058 | CD1 | ILE | B | 222 | 28.159 | 20.425 | 68.645 | 1.000 | 27.69 |
| ATOM | 4059 | CG2 | ILE | B | 222 | 28.131 | 23.351 | 68.293 | 1.000 | 33.22 |
| ATOM | 4060 | C   | ILE | B | 222 | 30.103 | 25.005 | 69.293 | 1.000 | 36.01 |
| ATOM | 4061 | O   | ILE | B | 222 | 30.270 | 25.723 | 68.300 | 1.000 | 32.03 |
| ATOM | 4062 | N   | GLN | B | 223 | 29.607 | 25.516 | 70.425 | 1.000 | 29.32 |
| ATOM | 4063 | CA  | GLN | B | 223 | 29.310 | 26.951 | 70.415 | 1.000 | 35.50 |
| ATOM | 4064 | CB  | GLN | B | 223 | 28.535 | 27.378 | 71.662 | 1.000 | 46.37 |
| ATOM | 4065 | CG  | GLN | B | 223 | 27.155 | 27.943 | 71.365 | 1.000 | 60.65 |
| ATOM | 4066 | CD  | GLN | B | 223 | 26.869 | 29.302 | 71.968 | 1.000 | 64.54 |
| ATOM | 4067 | OE1 | GLN | B | 223 | 27.164 | 30.353 | 71.390 | 1.000 | 52.88 |
| ATOM | 4068 | NE2 | GLN | B | 223 | 26.268 | 29.309 | 73.157 | 1.000 | 64.34 |
| ATOM | 4069 | C   | GLN | B | 223 | 30.601 | 27.759 | 70.275 | 1.000 | 32.82 |
| ATOM | 4070 | O   | GLN | B | 223 | 30.633 | 28.704 | 69.482 | 1.000 | 40.85 |
| ATOM | 4071 | N   | PHE | B | 224 | 31.643 | 27.396 | 71.019 | 1.000 | 25.74 |
| ATOM | 4072 | CA  | PHE | B | 224 | 32.907 | 28.131 | 70.963 | 1.000 | 27.71 |
| ATOM | 4073 | CB  | PHE | B | 224 | 33.949 | 27.479 | 71.869 | 1.000 | 24.79 |
| ATOM | 4074 | CG  | PHE | B | 224 | 35.314 | 28.117 | 71.858 | 1.000 | 25.53 |
| ATOM | 4075 | CD1 | PHE | B | 224 | 35.532 | 29.343 | 72.466 | 1.000 | 23.05 |
| ATOM | 4076 | CE1 | PHE | B | 224 | 36.785 | 29.925 | 72.476 | 1.000 | 27.91 |
| ATOM | 4077 | CZ  | PHE | B | 224 | 37.861 | 29.306 | 71.869 | 1.000 | 21.81 |
| ATOM | 4078 | CE2 | PHE | B | 224 | 37.654 | 28.086 | 71.253 | 1.000 | 21.78 |
| ATOM | 4079 | CD2 | PHE | B | 224 | 36.400 | 27.506 | 71.255 | 1.000 | 21.56 |
| ATOM | 4080 | C   | PHE | B | 224 | 33.441 | 28.175 | 69.535 | 1.000 | 25.15 |
| ATOM | 4081 | O   | PHE | B | 224 | 33.832 | 29.206 | 68.999 | 1.000 | 25.80 |
| ATOM | 4082 | N   | VAL | B | 225 | 33.454 | 27.006 | 68.903 | 1.000 | 26.67 |
| ATOM | 4083 | CA  | VAL | B | 225 | 33.933 | 26.919 | 67.532 | 1.000 | 29.86 |
| ATOM | 4084 | CB  | VAL | B | 225 | 33.999 | 25.467 | 67.029 | 1.000 | 20.12 |
| ATOM | 4085 | CG1 | VAL | B | 225 | 34.080 | 25.457 | 65.499 | 1.000 | 25.23 |
| ATOM | 4086 | CG2 | VAL | B | 225 | 35.171 | 24.740 | 67.654 | 1.000 | 26.39 |
| ATOM | 4087 | C   | VAL | B | 225 | 33.042 | 27.709 | 66.581 | 1.000 | 34.74 |
| ATOM | 4088 | O   | VAL | B | 225 | 33.545 | 28.329 | 65.644 | 1.000 | 35.87 |
| ATOM | 4089 | N   | ARG | B | 226 | 31.732 | 27.673 | 66.823 | 1.000 | 30.68 |
| ATOM | 4090 | CA  | ARG | B | 226 | 30.851 | 28.464 | 65.957 | 1.000 | 28.68 |
| ATOM | 4091 | CB  | ARG | B | 226 | 29.398 | 28.070 | 66.220 | 1.000 | 35.23 |
| ATOM | 4092 | CG  | ARG | B | 226 | 29.089 | 26.678 | 65.666 | 1.000 | 37.49 |
| ATOM | 4093 | CD  | ARG | B | 226 | 27.609 | 26.495 | 65.389 | 1.000 | 45.19 |
| ATOM | 4094 | NE  | ARG | B | 226 | 27.284 | 25.237 | 64.718 | 1.000 | 47.88 |
| ATOM | 4095 | CZ  | ARG | B | 226 | 26.232 | 24.481 | 65.025 | 1.000 | 52.72 |
| ATOM | 4096 | NH1 | ARG | B | 226 | 25.394 | 24.845 | 65.994 | 1.000 | 43.21 |
| ATOM | 4097 | NH2 | ARG | B | 226 | 26.003 | 23.348 | 64.369 | 1.000 | 42.49 |
| ATOM | 4098 | C   | ARG | B | 226 | 31.120 | 29.943 | 66.166 | 1.000 | 34.17 |
| ATOM | 4099 | O   | ARG | B | 226 | 31.166 | 30.741 | 65.228 | 1.000 | 36.74 |
| ATOM | 4100 | N   | THR | B | 227 | 31.340 | 30.366 | 67.409 | 1.000 | 28.96 |
| ATOM | 4101 | CA  | THR | B | 227 | 31.672 | 31.767 | 67.647 | 1.000 | 24.50 |
| ATOM | 4102 | CB  | THR | B | 227 | 31.786 | 32.029 | 69.165 | 1.000 | 34.83 |
| ATOM | 4103 | OG1 | THR | B | 227 | 30.553 | 31.661 | 69.790 | 1.000 | 51.39 |
| ATOM | 4104 | CG2 | THR | B | 227 | 32.011 | 33.502 | 69.440 | 1.000 | 28.79 |
| ATOM | 4105 | C   | THR | B | 227 | 32.980 | 32.179 | 66.987 | 1.000 | 26.81 |
| ATOM | 4106 | O   | THR | B | 227 | 33.096 | 33.245 | 66.375 | 1.000 | 44.96 |
| ATOM | 4107 | N   | VAL | B | 228 | 34.011 | 31.345 | 67.106 | 1.000 | 28.59 |

**FIGURE 85**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4108 | CA  | VAL | B | 228 | 35.306 | 31.681 | 66.512 | 1.000 | 31.86 |
| ATOM | 4109 | CB  | VAL | B | 228 | 36.413 | 30.705 | 66.949 | 1.000 | 36.11 |
| ATOM | 4110 | CG1 | VAL | B | 228 | 37.648 | 30.824 | 66.068 | 1.000 | 29.10 |
| ATOM | 4111 | CG2 | VAL | B | 228 | 36.821 | 30.927 | 68.408 | 1.000 | 24.69 |
| ATOM | 4112 | C   | VAL | B | 228 | 35.169 | 31.706 | 64.996 | 1.000 | 31.35 |
| ATOM | 4113 | O   | VAL | B | 228 | 35.760 | 32.543 | 64.321 | 1.000 | 23.32 |
| ATOM | 4114 | N   | ARG | B | 229 | 34.386 | 30.796 | 64.422 | 1.000 | 32.50 |
| ATOM | 4115 | CA  | ARG | B | 229 | 34.313 | 30.758 | 62.950 | 1.000 | 35.15 |
| ATOM | 4116 | CB  | ARG | B | 229 | 33.635 | 29.463 | 62.517 | 1.000 | 29.29 |
| ATOM | 4117 | CG  | ARG | B | 229 | 33.187 | 29.363 | 61.077 | 1.000 | 32.09 |
| ATOM | 4118 | CD  | ARG | B | 229 | 34.246 | 29.762 | 60.075 | 1.000 | 36.20 |
| ATOM | 4119 | NE  | ARG | B | 229 | 35.498 | 29.024 | 60.225 | 1.000 | 34.10 |
| ATOM | 4120 | CZ  | ARG | B | 229 | 36.530 | 29.145 | 59.398 | 1.000 | 31.12 |
| ATOM | 4121 | NH1 | ARG | B | 229 | 36.458 | 29.976 | 58.364 | 1.000 | 29.99 |
| ATOM | 4122 | NH2 | ARG | B | 229 | 37.637 | 28.440 | 59.603 | 1.000 | 25.49 |
| ATOM | 4123 | C   | ARG | B | 229 | 33.634 | 32.009 | 62.407 | 1.000 | 37.12 |
| ATOM | 4124 | O   | ARG | B | 229 | 34.041 | 32.534 | 61.363 | 1.000 | 38.65 |
| ATOM | 4125 | N   | ASP | B | 230 | 32.621 | 32.517 | 63.102 | 1.000 | 33.49 |
| ATOM | 4126 | CA  | ASP | B | 230 | 31.983 | 33.770 | 62.716 | 1.000 | 34.08 |
| ATOM | 4127 | CB  | ASP | B | 230 | 30.892 | 34.161 | 63.717 | 1.000 | 43.05 |
| ATOM | 4128 | CG  | ASP | B | 230 | 29.629 | 33.328 | 63.559 | 1.000 | 58.43 |
| ATOM | 4129 | OD1 | ASP | B | 230 | 29.284 | 32.975 | 62.409 | 1.000 | 90.62 |
| ATOM | 4130 | OD2 | ASP | B | 230 | 28.986 | 33.029 | 64.589 | 1.000 | 59.92 |
| ATOM | 4131 | C   | ASP | B | 230 | 32.996 | 34.899 | 62.621 | 1.000 | 32.94 |
| ATOM | 4132 | O   | ASP | B | 230 | 32.925 | 35.752 | 61.737 | 1.000 | 48.01 |
| ATOM | 4133 | N   | TYR | B | 231 | 33.967 | 34.941 | 63.537 | 1.000 | 28.38 |
| ATOM | 4134 | CA  | TYR | B | 231 | 34.903 | 36.062 | 63.457 | 1.000 | 31.35 |
| ATOM | 4135 | CB  | TYR | B | 231 | 35.624 | 36.312 | 64.779 | 1.000 | 33.15 |
| ATOM | 4136 | CG  | TYR | B | 231 | 34.805 | 37.080 | 65.791 | 1.000 | 35.44 |
| ATOM | 4137 | CD1 | TYR | B | 231 | 33.863 | 36.439 | 66.582 | 1.000 | 39.03 |
| ATOM | 4138 | CE1 | TYR | B | 231 | 33.119 | 37.148 | 67.508 | 1.000 | 45.49 |
| ATOM | 4139 | CZ  | TYR | B | 231 | 33.311 | 38.506 | 67.647 | 1.000 | 43.26 |
| ATOM | 4140 | OH  | TYR | B | 231 | 32.572 | 39.217 | 68.563 | 1.000 | 57.83 |
| ATOM | 4141 | CE2 | TYR | B | 231 | 34.240 | 39.164 | 66.874 | 1.000 | 37.85 |
| ATOM | 4142 | CD2 | TYR | B | 231 | 34.981 | 38.448 | 65.951 | 1.000 | 38.89 |
| ATOM | 4143 | C   | TYR | B | 231 | 35.937 | 35.836 | 62.358 | 1.000 | 32.28 |
| ATOM | 4144 | O   | TYR | B | 231 | 36.404 | 36.825 | 61.794 | 1.000 | 29.21 |
| ATOM | 4145 | N   | ILE | B | 232 | 36.288 | 34.583 | 62.079 | 1.000 | 29.70 |
| ATOM | 4146 | CA  | ILE | B | 232 | 37.274 | 34.317 | 61.032 | 1.000 | 26.08 |
| ATOM | 4147 | CB  | ILE | B | 232 | 37.731 | 32.855 | 60.956 | 1.000 | 26.12 |
| ATOM | 4148 | CG1 | ILE | B | 232 | 38.610 | 32.387 | 62.123 | 1.000 | 28.07 |
| ATOM | 4149 | CD1 | ILE | B | 232 | 38.492 | 30.888 | 62.342 | 1.000 | 30.24 |
| ATOM | 4150 | CG2 | ILE | B | 232 | 38.435 | 32.591 | 59.628 | 1.000 | 13.37 |
| ATOM | 4151 | C   | ILE | B | 232 | 36.664 | 34.713 | 59.686 | 1.000 | 24.35 |
| ATOM | 4152 | O   | ILE | B | 232 | 37.327 | 35.289 | 58.829 | 1.000 | 42.38 |
| ATOM | 4153 | N   | ASN | B | 233 | 35.384 | 34.401 | 59.536 | 1.000 | 24.49 |
| ATOM | 4154 | CA  | ASN | B | 233 | 34.678 | 34.774 | 58.310 | 1.000 | 35.31 |
| ATOM | 4155 | CB  | ASN | B | 233 | 33.288 | 34.125 | 58.331 | 1.000 | 33.92 |
| ATOM | 4156 | CG  | ASN | B | 233 | 33.411 | 32.644 | 58.011 | 1.000 | 35.63 |
| ATOM | 4157 | OD1 | ASN | B | 233 | 34.456 | 32.194 | 57.542 | 1.000 | 30.58 |
| ATOM | 4158 | ND2 | ASN | B | 233 | 32.353 | 31.889 | 58.275 | 1.000 | 39.02 |
| ATOM | 4159 | C   | ASN | B | 233 | 34.602 | 36.285 | 58.135 | 1.000 | 39.52 |

**FIGURE 86**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4160 | O   | ASN | B | 233 | 34.526 | 36.785 | 57.012 | 1.000 | 35.15 |
| ATOM | 4161 | N   | ARG | B | 234 | 34.636 | 37.051 | 59.217 | 1.000 | 38.25 |
| ATOM | 4162 | CA  | ARG | B | 234 | 34.605 | 38.501 | 59.186 | 1.000 | 36.43 |
| ATOM | 4163 | CB  | ARG | B | 234 | 33.826 | 39.055 | 60.391 | 1.000 | 49.91 |
| ATOM | 4164 | CG  | ARG | B | 234 | 32.397 | 38.562 | 60.514 | 1.000 | 60.74 |
| ATOM | 4165 | CD  | ARG | B | 234 | 31.528 | 39.486 | 61.349 | 1.000 | 58.98 |
| ATOM | 4166 | NE  | ARG | B | 234 | 30.847 | 38.790 | 62.440 | 1.000 | 54.26 |
| ATOM | 4167 | CZ  | ARG | B | 234 | 31.260 | 38.870 | 63.702 | 1.000 | 52.64 |
| ATOM | 4168 | NH1 | ARG | B | 234 | 32.325 | 39.608 | 63.990 | 1.000 | 52.91 |
| ATOM | 4169 | NH2 | ARG | B | 234 | 30.626 | 38.228 | 64.671 | 1.000 | 46.68 |
| ATOM | 4170 | C   | ARG | B | 234 | 35.998 | 39.117 | 59.211 | 1.000 | 33.22 |
| ATOM | 4171 | O   | ARG | B | 234 | 36.115 | 40.331 | 59.418 | 1.000 | 48.40 |
| ATOM | 4172 | N   | SER | B | 235 | 37.061 | 38.347 | 59.020 | 1.000 | 28.34 |
| ATOM | 4173 | CA  | SER | B | 235 | 38.421 | 38.885 | 59.043 | 1.000 | 32.54 |
| ATOM | 4174 | CB  | SER | B | 235 | 39.279 | 38.104 | 60.042 | 1.000 | 34.07 |
| ATOM | 4175 | OG  | SER | B | 235 | 38.666 | 38.004 | 61.314 | 1.000 | 34.54 |
| ATOM | 4176 | C   | SER | B | 235 | 39.076 | 38.841 | 57.671 | 1.000 | 40.54 |
| ATOM | 4177 | O   | SER | B | 235 | 40.079 | 38.152 | 57.421 | 1.000 | 36.22 |
| ATOM | 4178 | N   | PRO | B | 236 | 38.561 | 39.592 | 56.707 | 1.000 | 42.54 |
| ATOM | 4179 | CA  | PRO | B | 236 | 39.064 | 39.383 | 55.341 | 1.000 | 46.53 |
| ATOM | 4180 | CB  | PRO | B | 236 | 38.093 | 40.193 | 54.494 | 1.000 | 50.52 |
| ATOM | 4181 | CG  | PRO | B | 236 | 37.658 | 41.297 | 55.406 | 1.000 | 55.25 |
| ATOM | 4182 | CD  | PRO | B | 236 | 37.577 | 40.675 | 56.775 | 1.000 | 50.10 |
| ATOM | 4183 | C   | PRO | B | 236 | 40.491 | 39.914 | 55.278 | 1.000 | 45.59 |
| ATOM | 4184 | O   | PRO | B | 236 | 40.815 | 40.861 | 56.008 | 1.000 | 34.18 |
| ATOM | 4185 | N   | GLY | B | 237 | 41.304 | 39.292 | 54.422 | 1.000 | 33.61 |
| ATOM | 4186 | CA  | GLY | B | 237 | 42.692 | 39.734 | 54.313 | 1.000 | 30.68 |
| ATOM | 4187 | C   | GLY | B | 237 | 43.533 | 39.226 | 55.468 | 1.000 | 27.98 |
| ATOM | 4188 | O   | GLY | B | 237 | 44.720 | 39.537 | 55.554 | 1.000 | 36.96 |
| ATOM | 4189 | N   | ALA | B | 238 | 42.940 | 38.440 | 56.365 | 1.000 | 31.80 |
| ATOM | 4190 | CA  | ALA | B | 238 | 43.680 | 37.890 | 57.499 | 1.000 | 29.23 |
| ATOM | 4191 | CB  | ALA | B | 238 | 42.706 | 37.471 | 58.590 | 1.000 | 24.93 |
| ATOM | 4192 | C   | ALA | B | 238 | 44.543 | 36.705 | 57.090 | 1.000 | 29.82 |
| ATOM | 4193 | O   | ALA | B | 238 | 44.178 | 35.916 | 56.220 | 1.000 | 23.87 |
| ATOM | 4194 | N   | GLY | B | 239 | 45.703 | 36.544 | 57.722 | 1.000 | 26.54 |
| ATOM | 4195 | CA  | GLY | B | 239 | 46.486 | 35.346 | 57.425 | 1.000 | 26.69 |
| ATOM | 4196 | C   | GLY | B | 239 | 45.930 | 34.157 | 58.191 | 1.000 | 26.81 |
| ATOM | 4197 | O   | GLY | B | 239 | 44.747 | 34.100 | 58.534 | 1.000 | 29.92 |
| ATOM | 4198 | N   | PRO | B | 240 | 46.775 | 33.188 | 58.496 | 1.000 | 20.79 |
| ATOM | 4199 | CA  | PRO | B | 240 | 46.306 | 31.999 | 59.199 | 1.000 | 22.49 |
| ATOM | 4200 | CB  | PRO | B | 240 | 47.566 | 31.135 | 59.350 | 1.000 | 22.87 |
| ATOM | 4201 | CG  | PRO | B | 240 | 48.509 | 31.669 | 58.321 | 1.000 | 27.01 |
| ATOM | 4202 | CD  | PRO | B | 240 | 48.223 | 33.140 | 58.223 | 1.000 | 26.31 |
| ATOM | 4203 | C   | PRO | B | 240 | 45.763 | 32.328 | 60.583 | 1.000 | 25.93 |
| ATOM | 4204 | O   | PRO | B | 240 | 46.235 | 33.194 | 61.314 | 1.000 | 24.16 |
| ATOM | 4205 | N   | THR | B | 241 | 44.723 | 31.581 | 60.949 | 1.000 | 27.93 |
| ATOM | 4206 | CA  | THR | B | 241 | 44.224 | 31.620 | 62.317 | 1.000 | 18.48 |
| ATOM | 4207 | CB  | THR | B | 241 | 42.791 | 31.078 | 62.389 | 1.000 | 20.63 |
| ATOM | 4208 | OG1 | THR | B | 241 | 41.906 | 31.922 | 61.633 | 1.000 | 18.88 |
| ATOM | 4209 | CG2 | THR | B | 241 | 42.286 | 31.088 | 63.823 | 1.000 | 21.94 |
| ATOM | 4210 | C   | THR | B | 241 | 45.177 | 30.793 | 63.182 | 1.000 | 26.66 |
| ATOM | 4211 | O   | THR | B | 241 | 45.459 | 29.624 | 62.873 | 1.000 | 23.21 |

**FIGURE 87**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4212 | N   | VAL | B | 242 | 45.693 | 31.386 | 64.249 | 1.000 | 26.37 |
| ATOM | 4213 | CA  | VAL | B | 242 | 46.571 | 30.686 | 65.183 | 1.000 | 20.09 |
| ATOM | 4214 | CB  | VAL | B | 242 | 47.476 | 31.650 | 65.969 | 1.000 | 17.77 |
| ATOM | 4215 | CG1 | VAL | B | 242 | 47.993 | 30.997 | 67.245 | 1.000 | 24.64 |
| ATOM | 4216 | CG2 | VAL | B | 242 | 48.652 | 32.105 | 65.118 | 1.000 | 18.35 |
| ATOM | 4217 | C   | VAL | B | 242 | 45.745 | 29.871 | 66.171 | 1.000 | 21.82 |
| ATOM | 4218 | O   | VAL | B | 242 | 44.763 | 30.387 | 66.707 | 1.000 | 22.41 |
| ATOM | 4219 | N   | VAL | B | 243 | 46.124 | 28.618 | 66.415 | 1.000 | 24.38 |
| ATOM | 4220 | CA  | VAL | B | 243 | 45.444 | 27.807 | 67.426 | 1.000 | 16.94 |
| ATOM | 4221 | CB  | VAL | B | 243 | 44.512 | 26.759 | 66.797 | 1.000 | 22.95 |
| ATOM | 4222 | CG1 | VAL | B | 243 | 43.664 | 26.072 | 67.863 | 1.000 | 26.25 |
| ATOM | 4223 | CG2 | VAL | B | 243 | 43.612 | 27.396 | 65.744 | 1.000 | 15.21 |
| ATOM | 4224 | C   | VAL | B | 243 | 46.477 | 27.132 | 68.314 | 1.000 | 19.30 |
| ATOM | 4225 | O   | VAL | B | 243 | 47.444 | 26.568 | 67.807 | 1.000 | 19.80 |
| ATOM | 4226 | N   | HIS | B | 244 | 46.315 | 27.189 | 69.642 | 1.000 | 17.73 |
| ATOM | 4227 | CA  | HIS | B | 244 | 47.275 | 26.507 | 70.500 | 1.000 | 23.12 |
| ATOM | 4228 | CB  | HIS | B | 244 | 48.487 | 27.365 | 70.842 | 1.000 | 20.11 |
| ATOM | 4229 | CG  | HIS | B | 244 | 48.250 | 28.450 | 71.842 | 1.000 | 20.40 |
| ATOM | 4230 | ND1 | HIS | B | 244 | 48.315 | 28.263 | 73.200 | 1.000 | 23.45 |
| ATOM | 4231 | CE1 | HIS | B | 244 | 48.067 | 29.396 | 73.828 | 1.000 | 22.23 |
| ATOM | 4232 | NE2 | HIS | B | 244 | 47.850 | 30.330 | 72.921 | 1.000 | 22.87 |
| ATOM | 4233 | CD2 | HIS | B | 244 | 47.962 | 29.762 | 71.675 | 1.000 | 18.95 |
| ATOM | 4234 | C   | HIS | B | 244 | 46.582 | 26.046 | 71.783 | 1.000 | 26.22 |
| ATOM | 4235 | O   | HIS | B | 244 | 45.501 | 26.501 | 72.131 | 1.000 | 23.10 |
| ATOM | 4236 | N   | CYS | B | 245 | 47.252 | 25.119 | 72.440 | 1.000 | 22.02 |
| ATOM | 4237 | CA  | CYS | B | 245 | 46.907 | 24.642 | 73.777 | 1.000 | 19.58 |
| ATOM | 4238 | CB  | CYS | B | 245 | 46.233 | 23.282 | 73.751 | 1.000 | 24.57 |
| ATOM | 4239 | SG  | CYS | B | 245 | 47.070 | 21.959 | 72.834 | 1.000 | 28.98 |
| ATOM | 4240 | C   | CYS | B | 245 | 48.229 | 24.655 | 74.539 | 1.000 | 28.34 |
| ATOM | 4241 | O   | CYS | B | 245 | 48.948 | 25.667 | 74.457 | 1.000 | 29.70 |
| ATOM | 4242 | N   | SER | B | 246 | 48.559 | 23.571 | 75.231 | 1.000 | 25.71 |
| ATOM | 4243 | CA  | SER | B | 246 | 49.846 | 23.537 | 75.921 | 1.000 | 18.89 |
| ATOM | 4244 | CB  | SER | B | 246 | 49.839 | 22.627 | 77.146 | 1.000 | 23.17 |
| ATOM | 4245 | OG  | SER | B | 246 | 51.066 | 22.797 | 77.853 | 1.000 | 25.65 |
| ATOM | 4246 | C   | SER | B | 246 | 50.934 | 23.087 | 74.951 | 1.000 | 24.25 |
| ATOM | 4247 | O   | SER | B | 246 | 51.940 | 23.789 | 74.856 | 1.000 | 33.31 |
| ATOM | 4248 | N   | ALA | B | 247 | 50.731 | 21.962 | 74.259 | 1.000 | 18.83 |
| ATOM | 4249 | CA  | ALA | B | 247 | 51.743 | 21.518 | 73.314 | 1.000 | 15.18 |
| ATOM | 4250 | CB  | ALA | B | 247 | 52.036 | 20.041 | 73.514 | 1.000 | 17.96 |
| ATOM | 4251 | C   | ALA | B | 247 | 51.363 | 21.733 | 71.851 | 1.000 | 26.35 |
| ATOM | 4252 | O   | ALA | B | 247 | 52.187 | 21.474 | 70.959 | 1.000 | 31.41 |
| ATOM | 4253 | N   | GLY | B | 248 | 50.146 | 22.178 | 71.569 | 1.000 | 21.25 |
| ATOM | 4254 | CA  | GLY | B | 248 | 49.642 | 22.228 | 70.206 | 1.000 | 20.49 |
| ATOM | 4255 | C   | GLY | B | 248 | 49.312 | 20.840 | 69.659 | 1.000 | 30.46 |
| ATOM | 4256 | O   | GLY | B | 248 | 49.670 | 20.541 | 68.517 | 1.000 | 41.55 |
| ATOM | 4257 | N   | VAL | B | 249 | 48.635 | 19.983 | 70.414 | 1.000 | 28.50 |
| ATOM | 4258 | CA  | VAL | B | 249 | 48.393 | 18.586 | 70.073 | 1.000 | 34.64 |
| ATOM | 4259 | CB  | VAL | B | 249 | 49.048 | 17.670 | 71.137 | 1.000 | 36.74 |
| ATOM | 4260 | CG1 | VAL | B | 249 | 50.523 | 17.496 | 70.828 | 1.000 | 29.63 |
| ATOM | 4261 | CG2 | VAL | B | 249 | 48.858 | 18.238 | 72.545 | 1.000 | 30.44 |
| ATOM | 4262 | C   | VAL | B | 249 | 46.931 | 18.172 | 69.964 | 1.000 | 33.93 |
| ATOM | 4263 | O   | VAL | B | 249 | 46.301 | 18.395 | 68.930 | 1.000 | 40.05 |

**FIGURE 88**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4264 | N   | GLY | B | 250 | 46.392 | 17.537 | 71.003 | 1.000 | 28.29 |
| ATOM | 4265 | CA  | GLY | B | 250 | 45.069 | 16.957 | 71.039 | 1.000 | 22.14 |
| ATOM | 4266 | C   | GLY | B | 250 | 43.943 | 17.966 | 70.997 | 1.000 | 24.67 |
| ATOM | 4267 | O   | GLY | B | 250 | 43.137 | 17.979 | 70.063 | 1.000 | 30.05 |
| ATOM | 4268 | N   | ARG | B | 251 | 43.872 | 18.828 | 72.003 | 1.000 | 16.63 |
| ATOM | 4269 | CA  | ARG | B | 251 | 42.869 | 19.882 | 72.038 | 1.000 | 19.31 |
| ATOM | 4270 | CB  | ARG | B | 251 | 43.124 | 20.810 | 73.240 | 1.000 | 16.91 |
| ATOM | 4271 | CG  | ARG | B | 251 | 43.429 | 20.052 | 74.521 | 1.000 | 25.85 |
| ATOM | 4272 | CD  | ARG | B | 251 | 43.443 | 21.003 | 75.708 | 1.000 | 27.38 |
| ATOM | 4273 | NE  | ARG | B | 251 | 43.437 | 20.283 | 76.974 | 1.000 | 25.25 |
| ATOM | 4274 | CZ  | ARG | B | 251 | 43.500 | 20.852 | 78.167 | 1.000 | 28.05 |
| ATOM | 4275 | NH1 | ARG | B | 251 | 43.577 | 22.171 | 78.279 | 1.000 | 20.04 |
| ATOM | 4276 | NH2 | ARG | B | 251 | 43.485 | 20.081 | 79.246 | 1.000 | 33.27 |
| ATOM | 4277 | C   | ARG | B | 251 | 42.857 | 20.719 | 70.764 | 1.000 | 22.20 |
| ATOM | 4278 | O   | ARG | B | 251 | 41.814 | 20.925 | 70.142 | 1.000 | 37.10 |
| ATOM | 4279 | N   | THR | B | 252 | 44.023 | 21.228 | 70.372 | 1.000 | 25.42 |
| ATOM | 4280 | CA  | THR | B | 252 | 44.120 | 22.091 | 69.200 | 1.000 | 22.56 |
| ATOM | 4281 | CB  | THR | B | 252 | 45.571 | 22.546 | 68.965 | 1.000 | 23.97 |
| ATOM | 4282 | OG1 | THR | B | 252 | 45.903 | 23.531 | 69.956 | 1.000 | 25.35 |
| ATOM | 4283 | CG2 | THR | B | 252 | 45.734 | 23.196 | 67.600 | 1.000 | 15.93 |
| ATOM | 4284 | C   | THR | B | 252 | 43.631 | 21.357 | 67.965 | 1.000 | 20.90 |
| ATOM | 4285 | O   | THR | B | 252 | 42.825 | 21.833 | 67.170 | 1.000 | 27.79 |
| ATOM | 4286 | N   | GLY | B | 253 | 44.161 | 20.145 | 67.819 | 1.000 | 23.41 |
| ATOM | 4287 | CA  | GLY | B | 253 | 43.796 | 19.353 | 66.642 | 1.000 | 23.12 |
| ATOM | 4288 | C   | GLY | B | 253 | 42.313 | 19.031 | 66.705 | 1.000 | 28.00 |
| ATOM | 4289 | O   | GLY | B | 253 | 41.682 | 18.906 | 65.663 | 1.000 | 25.61 |
| ATOM | 4290 | N   | THR | B | 254 | 41.803 | 18.914 | 67.932 | 1.000 | 30.82 |
| ATOM | 4291 | CA  | THR | B | 254 | 40.382 | 18.631 | 68.136 | 1.000 | 28.89 |
| ATOM | 4292 | CB  | THR | B | 254 | 40.052 | 18.236 | 69.589 | 1.000 | 30.33 |
| ATOM | 4293 | OG1 | THR | B | 254 | 40.646 | 16.971 | 69.891 | 1.000 | 17.84 |
| ATOM | 4294 | CG2 | THR | B | 254 | 38.553 | 18.043 | 69.764 | 1.000 | 23.85 |
| ATOM | 4295 | C   | THR | B | 254 | 39.560 | 19.849 | 67.750 | 1.000 | 24.95 |
| ATOM | 4296 | O   | THR | B | 254 | 38.534 | 19.750 | 67.093 | 1.000 | 25.70 |
| ATOM | 4297 | N   | PHE | B | 255 | 40.023 | 21.033 | 68.168 | 1.000 | 20.14 |
| ATOM | 4298 | CA  | PHE | B | 255 | 39.330 | 22.238 | 67.761 | 1.000 | 18.66 |
| ATOM | 4299 | CB  | PHE | B | 255 | 40.055 | 23.472 | 68.309 | 1.000 | 20.98 |
| ATOM | 4300 | CG  | PHE | B | 255 | 39.468 | 24.795 | 67.891 | 1.000 | 25.32 |
| ATOM | 4301 | CD1 | PHE | B | 255 | 38.462 | 25.342 | 68.685 | 1.000 | 21.68 |
| ATOM | 4302 | CE1 | PHE | B | 255 | 37.893 | 26.550 | 68.349 | 1.000 | 20.94 |
| ATOM | 4303 | CZ  | PHE | B | 255 | 38.291 | 27.240 | 67.224 | 1.000 | 24.52 |
| ATOM | 4304 | CE2 | PHE | B | 255 | 39.287 | 26.713 | 66.419 | 1.000 | 22.92 |
| ATOM | 4305 | CD2 | PHE | B | 255 | 39.877 | 25.519 | 66.779 | 1.000 | 24.05 |
| ATOM | 4306 | C   | PHE | B | 255 | 39.255 | 22.352 | 66.239 | 1.000 | 20.18 |
| ATOM | 4307 | O   | PHE | B | 255 | 38.229 | 22.668 | 65.647 | 1.000 | 23.46 |
| ATOM | 4308 | N   | ILE | B | 256 | 40.401 | 22.192 | 65.592 | 1.000 | 14.95 |
| ATOM | 4309 | CA  | ILE | B | 256 | 40.468 | 22.444 | 64.155 | 1.000 | 19.23 |
| ATOM | 4310 | CB  | ILE | B | 256 | 41.923 | 22.480 | 63.668 | 1.000 | 24.98 |
| ATOM | 4311 | CG1 | ILE | B | 256 | 42.735 | 23.658 | 64.220 | 1.000 | 27.51 |
| ATOM | 4312 | CD1 | ILE | B | 256 | 44.198 | 23.613 | 63.833 | 1.000 | 28.76 |
| ATOM | 4313 | CG2 | ILE | B | 256 | 41.988 | 22.469 | 62.146 | 1.000 | 19.65 |
| ATOM | 4314 | C   | ILE | B | 256 | 39.642 | 21.413 | 63.395 | 1.000 | 21.66 |
| ATOM | 4315 | O   | ILE | B | 256 | 38.931 | 21.770 | 62.448 | 1.000 | 28.91 |

**FIGURE 89**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4316 | N   | ALA | B | 257 | 39.699 | 20.142 | 63.782 | 1.000 | 18.05 |
| ATOM | 4317 | CA  | ALA | B | 257 | 38.802 | 19.169 | 63.158 | 1.000 | 19.47 |
| ATOM | 4318 | CB  | ALA | B | 257 | 38.987 | 17.798 | 63.775 | 1.000 | 21.30 |
| ATOM | 4319 | C   | ALA | B | 257 | 37.346 | 19.600 | 63.303 | 1.000 | 24.28 |
| ATOM | 4320 | O   | ALA | B | 257 | 36.588 | 19.578 | 62.335 | 1.000 | 29.52 |
| ATOM | 4321 | N   | LEU | B | 258 | 36.913 | 19.998 | 64.506 | 1.000 | 19.55 |
| ATOM | 4322 | CA  | LEU | B | 258 | 35.511 | 20.383 | 64.656 | 1.000 | 23.44 |
| ATOM | 4323 | CB  | LEU | B | 258 | 35.187 | 20.725 | 66.109 | 1.000 | 26.54 |
| ATOM | 4324 | CG  | LEU | B | 258 | 33.718 | 21.043 | 66.402 | 1.000 | 26.93 |
| ATOM | 4325 | CD1 | LEU | B | 258 | 32.830 | 19.879 | 65.989 | 1.000 | 33.89 |
| ATOM | 4326 | CD2 | LEU | B | 258 | 33.523 | 21.383 | 67.874 | 1.000 | 26.13 |
| ATOM | 4327 | C   | LEU | B | 258 | 35.162 | 21.561 | 63.747 | 1.000 | 26.19 |
| ATOM | 4328 | O   | LEU | B | 258 | 34.104 | 21.555 | 63.113 | 1.000 | 34.02 |
| ATOM | 4329 | N   | ASP | B | 259 | 36.047 | 22.546 | 63.699 | 1.000 | 24.40 |
| ATOM | 4330 | CA  | ASP | B | 259 | 35.925 | 23.714 | 62.834 | 1.000 | 27.44 |
| ATOM | 4331 | CB  | ASP | B | 259 | 37.184 | 24.585 | 62.907 | 1.000 | 26.51 |
| ATOM | 4332 | CG  | ASP | B | 259 | 37.015 | 25.907 | 62.185 | 1.000 | 31.73 |
| ATOM | 4333 | OD1 | ASP | B | 259 | 35.871 | 26.400 | 62.144 | 1.000 | 33.45 |
| ATOM | 4334 | OD2 | ASP | B | 259 | 38.013 | 26.448 | 61.664 | 1.000 | 25.69 |
| ATOM | 4335 | C   | ASP | B | 259 | 35.678 | 23.286 | 61.392 | 1.000 | 22.95 |
| ATOM | 4336 | O   | ASP | B | 259 | 34.813 | 23.822 | 60.702 | 1.000 | 30.45 |
| ATOM | 4337 | N   | ARG | B | 260 | 36.446 | 22.302 | 60.950 | 1.000 | 26.62 |
| ATOM | 4338 | CA  | ARG | B | 260 | 36.361 | 21.798 | 59.585 | 1.000 | 33.18 |
| ATOM | 4339 | CB  | ARG | B | 260 | 37.519 | 20.835 | 59.319 | 1.000 | 31.29 |
| ATOM | 4340 | CG  | ARG | B | 260 | 38.785 | 21.473 | 58.778 | 1.000 | 30.70 |
| ATOM | 4341 | CD  | ARG | B | 260 | 39.239 | 20.700 | 57.536 | 1.000 | 37.95 |
| ATOM | 4342 | NE  | ARG | B | 260 | 40.673 | 20.498 | 57.556 | 1.000 | 41.13 |
| ATOM | 4343 | CZ  | ARG | B | 260 | 41.391 | 19.709 | 56.782 | 1.000 | 33.80 |
| ATOM | 4344 | NH1 | ARG | B | 260 | 40.798 | 18.979 | 55.856 | 1.000 | 42.79 |
| ATOM | 4345 | NH2 | ARG | B | 260 | 42.705 | 19.660 | 56.957 | 1.000 | 37.06 |
| ATOM | 4346 | C   | ARG | B | 260 | 35.055 | 21.066 | 59.301 | 1.000 | 38.95 |
| ATOM | 4347 | O   | ARG | B | 260 | 34.398 | 21.344 | 58.296 | 1.000 | 34.89 |
| ATOM | 4348 | N   | ILE | B | 261 | 34.673 | 20.123 | 60.157 | 1.000 | 40.78 |
| ATOM | 4349 | CA  | ILE | B | 261 | 33.506 | 19.282 | 59.888 | 1.000 | 36.65 |
| ATOM | 4350 | CB  | ILE | B | 261 | 33.512 | 18.013 | 60.759 | 1.000 | 36.83 |
| ATOM | 4351 | CG1 | ILE | B | 261 | 33.172 | 18.232 | 62.236 | 1.000 | 36.37 |
| ATOM | 4352 | CD1 | ILE | B | 261 | 33.788 | 17.170 | 63.128 | 1.000 | 27.30 |
| ATOM | 4353 | CG2 | ILE | B | 261 | 34.851 | 17.297 | 60.648 | 1.000 | 30.19 |
| ATOM | 4354 | C   | ILE | B | 261 | 32.193 | 20.033 | 60.076 | 1.000 | 37.68 |
| ATOM | 4355 | O   | ILE | B | 261 | 31.233 | 19.779 | 59.332 | 1.000 | 29.23 |
| ATOM | 4356 | N   | LEU | B | 262 | 32.121 | 20.960 | 61.032 | 1.000 | 29.30 |
| ATOM | 4357 | CA  | LEU | B | 262 | 30.910 | 21.778 | 61.134 | 1.000 | 34.05 |
| ATOM | 4358 | CB  | LEU | B | 262 | 30.909 | 22.676 | 62.372 | 1.000 | 34.84 |
| ATOM | 4359 | CG  | LEU | B | 262 | 30.865 | 21.951 | 63.722 | 1.000 | 33.81 |
| ATOM | 4360 | CD1 | LEU | B | 262 | 30.907 | 22.931 | 64.886 | 1.000 | 29.40 |
| ATOM | 4361 | CD2 | LEU | B | 262 | 29.628 | 21.067 | 63.813 | 1.000 | 31.05 |
| ATOM | 4362 | C   | LEU | B | 262 | 30.763 | 22.639 | 59.882 | 1.000 | 49.12 |
| ATOM | 4363 | O   | LEU | B | 262 | 29.667 | 23.081 | 59.538 | 1.000 | 56.67 |
| ATOM | 4364 | N   | GLN | B | 263 | 31.888 | 22.887 | 59.204 | 1.000 | 44.18 |
| ATOM | 4365 | CA  | GLN | B | 263 | 31.808 | 23.682 | 57.982 | 1.000 | 46.28 |
| ATOM | 4366 | CB  | GLN | B | 263 | 33.169 | 24.218 | 57.542 | 1.000 | 42.43 |
| ATOM | 4367 | CG  | GLN | B | 263 | 33.463 | 25.604 | 58.110 | 1.000 | 37.21 |

**FIGURE 90**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |        |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|--------|
| ATOM | 4368 | CD  | GLN | B | 263 | 34.905 | 25.991 | 57.847 | 1.000 | 38.82  |
| ATOM | 4369 | OE1 | GLN | B | 263 | 35.200 | 26.564 | 56.803 | 1.000 | 42.28  |
| ATOM | 4370 | NE2 | GLN | B | 263 | 35.789 | 25.670 | 58.782 | 1.000 | 38.53  |
| ATOM | 4371 | C   | GLN | B | 263 | 31.207 | 22.830 | 56.870 | 1.000 | 43.95  |
| ATOM | 4372 | O   | GLN | B | 263 | 30.412 | 23.325 | 56.083 | 1.000 | 46.04  |
| ATOM | 4373 | N   | GLN | B | 264 | 31.609 | 21.563 | 56.843 | 1.000 | 40.32  |
| ATOM | 4374 | CA  | GLN | B | 264 | 31.058 | 20.637 | 55.859 | 1.000 | 43.58  |
| ATOM | 4375 | CB  | GLN | B | 264 | 31.776 | 19.291 | 55.904 | 1.000 | 41.24  |
| ATOM | 4376 | CG  | GLN | B | 264 | 33.299 | 19.353 | 55.893 | 1.000 | 32.42  |
| ATOM | 4377 | CD  | GLN | B | 264 | 33.885 | 17.975 | 56.138 | 1.000 | 34.83  |
| ATOM | 4378 | OE1 | GLN | B | 264 | 33.154 | 16.982 | 56.114 | 1.000 | 49.05  |
| ATOM | 4379 | NE2 | GLN | B | 264 | 35.181 | 17.880 | 56.386 | 1.000 | 36.65  |
| ATOM | 4380 | C   | GLN | B | 264 | 29.557 | 20.453 | 56.088 | 1.000 | 46.84  |
| ATOM | 4381 | O   | GLN | B | 264 | 28.787 | 20.463 | 55.125 | 1.000 | 60.95  |
| ATOM | 4382 | N   | LEU | B | 265 | 29.143 | 20.293 | 57.339 | 1.000 | 44.06  |
| ATOM | 4383 | CA  | LEU | B | 265 | 27.744 | 20.092 | 57.689 | 1.000 | 48.45  |
| ATOM | 4384 | CB  | LEU | B | 265 | 27.541 | 20.198 | 59.204 | 1.000 | 48.90  |
| ATOM | 4385 | CG  | LEU | B | 265 | 28.027 | 19.015 | 60.044 | 1.000 | 49.51  |
| ATOM | 4386 | CD1 | LEU | B | 265 | 27.374 | 19.048 | 61.416 | 1.000 | 39.17  |
| ATOM | 4387 | CD2 | LEU | B | 265 | 27.761 | 17.702 | 59.326 | 1.000 | 46.39  |
| ATOM | 4388 | C   | LEU | B | 265 | 26.816 | 21.098 | 57.009 | 1.000 | 55.29  |
| ATOM | 4389 | O   | LEU | B | 265 | 25.738 | 20.747 | 56.529 | 1.000 | 61.57  |
| ATOM | 4390 | N   | ASP | B | 266 | 27.242 | 22.353 | 56.989 | 1.000 | 56.37  |
| ATOM | 4391 | CA  | ASP | B | 266 | 26.489 | 23.438 | 56.374 | 1.000 | 56.13  |
| ATOM | 4392 | CB  | ASP | B | 266 | 26.708 | 24.734 | 57.154 | 1.000 | 62.09  |
| ATOM | 4393 | CG  | ASP | B | 266 | 26.306 | 24.619 | 58.612 | 1.000 | 68.79  |
| ATOM | 4394 | OD1 | ASP | B | 266 | 25.108 | 24.405 | 58.894 | 1.000 | 79.54  |
| ATOM | 4395 | OD2 | ASP | B | 266 | 27.190 | 24.742 | 59.489 | 1.000 | 81.01  |
| ATOM | 4396 | C   | ASP | B | 266 | 26.905 | 23.610 | 54.917 | 1.000 | 50.88  |
| ATOM | 4397 | O   | ASP | B | 266 | 26.597 | 24.607 | 54.265 | 1.000 | 58.84  |
| ATOM | 4398 | N   | SER | B | 267 | 27.632 | 22.622 | 54.407 | 1.000 | 53.13  |
| ATOM | 4399 | CA  | SER | B | 267 | 28.177 | 22.699 | 53.056 | 1.000 | 64.34  |
| ATOM | 4400 | CB  | SER | B | 267 | 29.708 | 22.798 | 53.101 | 1.000 | 56.46  |
| ATOM | 4401 | OG  | SER | B | 267 | 30.143 | 24.108 | 52.784 | 1.000 | 60.08  |
| ATOM | 4402 | C   | SER | B | 267 | 27.759 | 21.499 | 52.214 | 1.000 | 75.07  |
| ATOM | 4403 | O   | SER | B | 267 | 26.653 | 21.444 | 51.677 | 1.000 | 79.48  |
| ATOM | 4404 | N   | LYS | B | 268 | 28.656 | 20.523 | 52.092 | 1.000 | 83.42  |
| ATOM | 4405 | CA  | LYS | B | 268 | 28.385 | 19.358 | 51.257 | 1.000 | 86.00  |
| ATOM | 4406 | CB  | LYS | B | 268 | 29.664 | 18.545 | 51.050 | 1.000 | 90.22  |
| ATOM | 4407 | CG  | LYS | B | 268 | 30.899 | 19.402 | 50.804 | 1.000 | 90.85  |
| ATOM | 4408 | CD  | LYS | B | 268 | 31.608 | 19.724 | 52.110 | 1.000 | 87.44  |
| ATOM | 4409 | CE  | LYS | B | 268 | 32.908 | 20.484 | 51.868 | 1.000 | 87.50  |
| ATOM | 4410 | NZ  | LYS | B | 268 | 33.982 | 19.590 | 51.340 | 1.000 | 90.86  |
| ATOM | 4411 | C   | LYS | B | 268 | 27.279 | 18.493 | 51.854 | 1.000 | 79.53  |
| ATOM | 4412 | O   | LYS | B | 268 | 26.697 | 18.840 | 52.883 | 1.000 | 65.16  |
| ATOM | 4413 | N   | ASP | B | 269 | 27.000 | 17.380 | 51.183 | 1.000 | 75.19  |
| ATOM | 4414 | CA  | ASP | B | 269 | 25.948 | 16.453 | 51.576 | 1.000 | 74.46  |
| ATOM | 4415 | CB  | ASP | B | 269 | 25.390 | 15.742 | 50.342 | 1.000 | 83.40  |
| ATOM | 4416 | CG  | ASP | B | 269 | 25.381 | 16.633 | 49.114 | 1.000 | 92.95  |
| ATOM | 4417 | OD1 | ASP | B | 269 | 24.301 | 16.816 | 48.509 | 1.000 | 99.02  |
| ATOM | 4418 | OD2 | ASP | B | 269 | 26.460 | 17.153 | 48.752 | 1.000 | 105.13 |
| ATOM | 4419 | C   | ASP | B | 269 | 26.475 | 15.440 | 52.584 | 1.000 | 69.56  |

**FIGURE 91**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4420 | O   | ASP | B | 269 | 25.755 | 14.571 | 53.071 | 1.000 | 66.15 |
| ATOM | 4421 | N   | SER | B | 270 | 27.763 | 15.573 | 52.883 | 1.000 | 63.01 |
| ATOM | 4422 | CA  | SER | B | 270 | 28.449 | 14.658 | 53.782 | 1.000 | 53.77 |
| ATOM | 4423 | CB  | SER | B | 270 | 29.261 | 13.633 | 52.991 | 1.000 | 58.45 |
| ATOM | 4424 | OG  | SER | B | 270 | 30.230 | 12.983 | 53.797 | 1.000 | 73.26 |
| ATOM | 4425 | C   | SER | B | 270 | 29.357 | 15.436 | 54.734 | 1.000 | 46.99 |
| ATOM | 4426 | O   | SER | B | 270 | 29.393 | 16.664 | 54.654 | 1.000 | 42.15 |
| ATOM | 4427 | N   | VAL | B | 271 | 30.035 | 14.690 | 55.588 | 1.000 | 48.78 |
| ATOM | 4428 | CA  | VAL | B | 271 | 31.029 | 15.141 | 56.544 | 1.000 | 48.00 |
| ATOM | 4429 | CB  | VAL | B | 271 | 30.446 | 15.379 | 57.946 | 1.000 | 49.59 |
| ATOM | 4430 | CG1 | VAL | B | 271 | 29.390 | 14.335 | 58.283 | 1.000 | 49.18 |
| ATOM | 4431 | CG2 | VAL | B | 271 | 31.569 | 15.369 | 58.980 | 1.000 | 36.94 |
| ATOM | 4432 | C   | VAL | B | 271 | 32.145 | 14.100 | 56.637 | 1.000 | 42.78 |
| ATOM | 4433 | O   | VAL | B | 271 | 31.864 | 12.911 | 56.794 | 1.000 | 49.77 |
| ATOM | 4434 | N   | ASP | B | 272 | 33.390 | 14.532 | 56.524 | 1.000 | 38.85 |
| ATOM | 4435 | CA  | ASP | B | 272 | 34.530 | 13.630 | 56.527 | 1.000 | 35.40 |
| ATOM | 4436 | CB  | ASP | B | 272 | 35.438 | 13.862 | 55.314 | 1.000 | 27.29 |
| ATOM | 4437 | CG  | ASP | B | 272 | 36.212 | 12.617 | 54.924 | 1.000 | 35.62 |
| ATOM | 4438 | OD1 | ASP | B | 272 | 36.101 | 11.583 | 55.615 | 1.000 | 37.07 |
| ATOM | 4439 | OD2 | ASP | B | 272 | 36.947 | 12.666 | 53.915 | 1.000 | 50.42 |
| ATOM | 4440 | C   | ASP | B | 272 | 35.359 | 13.795 | 57.792 | 1.000 | 40.21 |
| ATOM | 4441 | O   | ASP | B | 272 | 36.364 | 14.503 | 57.797 | 1.000 | 41.63 |
| ATOM | 4442 | N   | ILE | B | 273 | 34.929 | 13.131 | 58.862 | 1.000 | 40.79 |
| ATOM | 4443 | CA  | ILE | B | 273 | 35.679 | 13.285 | 60.108 | 1.000 | 34.29 |
| ATOM | 4444 | CB  | ILE | B | 273 | 34.909 | 12.721 | 61.310 | 1.000 | 30.34 |
| ATOM | 4445 | CG1 | ILE | B | 273 | 33.565 | 13.409 | 61.576 | 1.000 | 31.83 |
| ATOM | 4446 | CD1 | ILE | B | 273 | 32.766 | 12.740 | 62.679 | 1.000 | 27.01 |
| ATOM | 4447 | CG2 | ILE | B | 273 | 35.768 | 12.761 | 62.563 | 1.000 | 28.54 |
| ATOM | 4448 | C   | ILE | B | 273 | 37.053 | 12.639 | 59.968 | 1.000 | 39.35 |
| ATOM | 4449 | O   | ILE | B | 273 | 38.060 | 13.284 | 60.295 | 1.000 | 37.96 |
| ATOM | 4450 | N   | TYR | B | 274 | 37.080 | 11.404 | 59.482 | 1.000 | 40.06 |
| ATOM | 4451 | CA  | TYR | B | 274 | 38.320 | 10.692 | 59.209 | 1.000 | 36.37 |
| ATOM | 4452 | CB  | TYR | B | 274 | 38.083 | 9.343  | 58.534 | 1.000 | 34.20 |
| ATOM | 4453 | CG  | TYR | B | 274 | 39.288 | 8.485  | 58.221 | 1.000 | 26.44 |
| ATOM | 4454 | CD1 | TYR | B | 274 | 39.691 | 7.499  | 59.115 | 1.000 | 29.38 |
| ATOM | 4455 | CE1 | TYR | B | 274 | 40.787 | 6.698  | 58.847 | 1.000 | 34.20 |
| ATOM | 4456 | CZ  | TYR | B | 274 | 41.501 | 6.863  | 57.683 | 1.000 | 32.34 |
| ATOM | 4457 | OH  | TYR | B | 274 | 42.595 | 6.077  | 57.401 | 1.000 | 45.24 |
| ATOM | 4458 | CE2 | TYR | B | 274 | 41.126 | 7.829  | 56.774 | 1.000 | 32.36 |
| ATOM | 4459 | CD2 | TYR | B | 274 | 40.033 | 8.609  | 57.056 | 1.000 | 26.39 |
| ATOM | 4460 | C   | TYR | B | 274 | 39.228 | 11.528 | 58.299 | 1.000 | 32.63 |
| ATOM | 4461 | O   | TYR | B | 274 | 40.436 | 11.567 | 58.534 | 1.000 | 31.00 |
| ATOM | 4462 | N   | GLY | B | 275 | 38.634 | 12.102 | 57.266 | 1.000 | 39.31 |
| ATOM | 4463 | CA  | GLY | B | 275 | 39.375 | 12.824 | 56.239 | 1.000 | 35.88 |
| ATOM | 4464 | C   | GLY | B | 275 | 40.102 | 14.006 | 56.865 | 1.000 | 40.67 |
| ATOM | 4465 | O   | GLY | B | 275 | 41.263 | 14.270 | 56.555 | 1.000 | 33.84 |
| ATOM | 4466 | N   | ALA | B | 276 | 39.376 | 14.679 | 57.751 | 1.000 | 36.51 |
| ATOM | 4467 | CA  | ALA | B | 276 | 39.906 | 15.849 | 58.442 | 1.000 | 37.26 |
| ATOM | 4468 | CB  | ALA | B | 276 | 38.791 | 16.511 | 59.244 | 1.000 | 29.45 |
| ATOM | 4469 | C   | ALA | B | 276 | 41.097 | 15.502 | 59.323 | 1.000 | 31.12 |
| ATOM | 4470 | O   | ALA | B | 276 | 42.147 | 16.150 | 59.234 | 1.000 | 27.41 |
| ATOM | 4471 | N   | VAL | B | 277 | 40.972 | 14.480 | 60.169 | 1.000 | 28.39 |

**FIGURE 92**



Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4472 | CA  | VAL | B | 277 | 42.049 | 14.164 | 61.101 | 1.000 | 26.25 |
| ATOM | 4473 | CB  | VAL | B | 277 | 41.639 | 13.101 | 62.138 | 1.000 | 27.10 |
| ATOM | 4474 | CG1 | VAL | B | 277 | 42.882 | 12.558 | 62.827 | 1.000 | 24.03 |
| ATOM | 4475 | CG2 | VAL | B | 277 | 40.671 | 13.681 | 63.159 | 1.000 | 28.27 |
| ATOM | 4476 | C   | VAL | B | 277 | 43.306 | 13.654 | 60.402 | 1.000 | 31.14 |
| ATOM | 4477 | O   | VAL | B | 277 | 44.411 | 13.880 | 60.897 | 1.000 | 29.79 |
| ATOM | 4478 | N   | HIS | B | 278 | 43.121 | 12.975 | 59.277 | 1.000 | 27.18 |
| ATOM | 4479 | CA  | HIS | B | 278 | 44.202 | 12.495 | 58.431 | 1.000 | 25.97 |
| ATOM | 4480 | CB  | HIS | B | 278 | 43.601 | 11.645 | 57.309 | 1.000 | 33.39 |
| ATOM | 4481 | CG  | HIS | B | 278 | 44.609 | 11.055 | 56.378 | 1.000 | 34.11 |
| ATOM | 4482 | ND1 | HIS | B | 278 | 45.201 | 11.773 | 55.367 | 1.000 | 25.09 |
| ATOM | 4483 | CE1 | HIS | B | 278 | 46.048 | 11.002 | 54.708 | 1.000 | 28.44 |
| ATOM | 4484 | NE2 | HIS | B | 278 | 46.026 | 9.801  | 55.267 | 1.000 | 31.16 |
| ATOM | 4485 | CD2 | HIS | B | 278 | 45.138 | 9.806  | 56.307 | 1.000 | 31.49 |
| ATOM | 4486 | C   | HIS | B | 278 | 45.001 | 13.660 | 57.859 | 1.000 | 24.46 |
| ATOM | 4487 | O   | HIS | B | 278 | 46.225 | 13.753 | 57.928 | 1.000 | 25.14 |
| ATOM | 4488 | N   | ASP | B | 279 | 44.283 | 14.603 | 57.260 | 1.000 | 23.15 |
| ATOM | 4489 | CA  | ASP | B | 279 | 44.887 | 15.817 | 56.715 | 1.000 | 24.67 |
| ATOM | 4490 | CB  | ASP | B | 279 | 43.776 | 16.718 | 56.178 | 1.000 | 29.92 |
| ATOM | 4491 | CG  | ASP | B | 279 | 44.160 | 17.578 | 55.001 | 1.000 | 37.07 |
| ATOM | 4492 | OD1 | ASP | B | 279 | 45.077 | 17.212 | 54.235 | 1.000 | 38.06 |
| ATOM | 4493 | OD2 | ASP | B | 279 | 43.537 | 18.648 | 54.835 | 1.000 | 30.88 |
| ATOM | 4494 | C   | ASP | B | 279 | 45.706 | 16.530 | 57.784 | 1.000 | 25.54 |
| ATOM | 4495 | O   | ASP | B | 279 | 46.843 | 16.941 | 57.550 | 1.000 | 21.93 |
| ATOM | 4496 | N   | LEU | B | 280 | 45.150 | 16.673 | 58.991 | 1.000 | 18.66 |
| ATOM | 4497 | CA  | LEU | B | 280 | 45.867 | 17.373 | 60.061 | 1.000 | 27.59 |
| ATOM | 4498 | CB  | LEU | B | 280 | 45.025 | 17.491 | 61.331 | 1.000 | 23.76 |
| ATOM | 4499 | CG  | LEU | B | 280 | 43.732 | 18.302 | 61.281 | 1.000 | 29.33 |
| ATOM | 4500 | CD1 | LEU | B | 280 | 43.374 | 18.821 | 62.668 | 1.000 | 34.75 |
| ATOM | 4501 | CD2 | LEU | B | 280 | 43.836 | 19.450 | 60.293 | 1.000 | 30.06 |
| ATOM | 4502 | C   | LEU | B | 280 | 47.181 | 16.678 | 60.432 | 1.000 | 33.16 |
| ATOM | 4503 | O   | LEU | B | 280 | 48.218 | 17.326 | 60.576 | 1.000 | 22.56 |
| ATOM | 4504 | N   | ARG | B | 281 | 47.077 | 15.363 | 60.589 | 1.000 | 29.37 |
| ATOM | 4505 | CA  | ARG | B | 281 | 48.168 | 14.491 | 60.979 | 1.000 | 31.07 |
| ATOM | 4506 | CB  | ARG | B | 281 | 47.675 | 13.042 | 61.092 | 1.000 | 28.63 |
| ATOM | 4507 | CG  | ARG | B | 281 | 46.655 | 12.833 | 62.199 | 1.000 | 26.35 |
| ATOM | 4508 | CD  | ARG | B | 281 | 47.328 | 12.460 | 63.506 | 1.000 | 27.07 |
| ATOM | 4509 | NE  | ARG | B | 281 | 46.350 | 12.116 | 64.535 | 1.000 | 30.18 |
| ATOM | 4510 | CZ  | ARG | B | 281 | 46.041 | 10.880 | 64.893 | 1.000 | 27.85 |
| ATOM | 4511 | NH1 | ARG | B | 281 | 46.628 | 9.852  | 64.310 | 1.000 | 31.06 |
| ATOM | 4512 | NH2 | ARG | B | 281 | 45.138 | 10.667 | 65.838 | 1.000 | 39.11 |
| ATOM | 4513 | C   | ARG | B | 281 | 49.318 | 14.561 | 59.985 | 1.000 | 29.17 |
| ATOM | 4514 | O   | ARG | B | 281 | 50.478 | 14.363 | 60.347 | 1.000 | 28.56 |
| ATOM | 4515 | N   | LEU | B | 282 | 48.986 | 14.842 | 58.727 | 1.000 | 30.67 |
| ATOM | 4516 | CA  | LEU | B | 282 | 50.041 | 15.001 | 57.727 | 1.000 | 30.29 |
| ATOM | 4517 | CB  | LEU | B | 282 | 49.455 | 15.139 | 56.327 | 1.000 | 24.52 |
| ATOM | 4518 | CG  | LEU | B | 282 | 48.830 | 13.899 | 55.689 | 1.000 | 27.65 |
| ATOM | 4519 | CD1 | LEU | B | 282 | 48.201 | 14.290 | 54.357 | 1.000 | 22.99 |
| ATOM | 4520 | CD2 | LEU | B | 282 | 49.859 | 12.792 | 55.511 | 1.000 | 27.48 |
| ATOM | 4521 | C   | LEU | B | 282 | 50.913 | 16.222 | 58.014 | 1.000 | 27.27 |
| ATOM | 4522 | O   | LEU | B | 282 | 52.030 | 16.277 | 57.506 | 1.000 | 26.46 |
| ATOM | 4523 | N   | HIS | B | 283 | 50.418 | 17.178 | 58.794 | 1.000 | 26.63 |

**FIGURE 93**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4524 | CA  | HIS | B | 283 | 51.104 | 18.459 | 58.962 | 1.000 | 28.55 |
| ATOM | 4525 | CB  | HIS | B | 283 | 50.157 | 19.615 | 58.551 | 1.000 | 26.78 |
| ATOM | 4526 | CG  | HIS | B | 283 | 49.852 | 19.437 | 57.083 | 1.000 | 31.38 |
| ATOM | 4527 | ND1 | HIS | B | 283 | 50.669 | 19.906 | 56.078 | 1.000 | 29.31 |
| ATOM | 4528 | CE1 | HIS | B | 283 | 50.164 | 19.584 | 54.901 | 1.000 | 26.22 |
| ATOM | 4529 | NE2 | HIS | B | 283 | 49.048 | 18.905 | 55.114 | 1.000 | 26.82 |
| ATOM | 4530 | CD2 | HIS | B | 283 | 48.838 | 18.792 | 56.461 | 1.000 | 28.69 |
| ATOM | 4531 | C   | HIS | B | 283 | 51.658 | 18.636 | 60.359 | 1.000 | 26.35 |
| ATOM | 4532 | O   | HIS | B | 283 | 52.552 | 19.465 | 60.565 | 1.000 | 24.96 |
| ATOM | 4533 | N   | ARG | B | 284 | 51.186 | 17.858 | 61.335 | 1.000 | 20.29 |
| ATOM | 4534 | CA  | ARG | B | 284 | 51.798 | 17.980 | 62.664 | 1.000 | 21.12 |
| ATOM | 4535 | CB  | ARG | B | 284 | 51.322 | 19.245 | 63.391 | 1.000 | 20.38 |
| ATOM | 4536 | CG  | ARG | B | 284 | 52.150 | 19.588 | 64.639 | 1.000 | 22.36 |
| ATOM | 4537 | CD  | ARG | B | 284 | 51.699 | 20.875 | 65.292 | 1.000 | 21.53 |
| ATOM | 4538 | NE  | ARG | B | 284 | 52.054 | 21.061 | 66.698 | 1.000 | 19.46 |
| ATOM | 4539 | CZ  | ARG | B | 284 | 53.142 | 21.705 | 67.107 | 1.000 | 25.24 |
| ATOM | 4540 | NH1 | ARG | B | 284 | 54.004 | 22.225 | 66.238 | 1.000 | 24.69 |
| ATOM | 4541 | NH2 | ARG | B | 284 | 53.412 | 21.850 | 68.402 | 1.000 | 27.97 |
| ATOM | 4542 | C   | ARG | B | 284 | 51.493 | 16.731 | 63.482 | 1.000 | 16.74 |
| ATOM | 4543 | O   | ARG | B | 284 | 50.383 | 16.207 | 63.410 | 1.000 | 20.61 |
| ATOM | 4544 | N   | VAL | B | 285 | 52.454 | 16.252 | 64.253 | 1.000 | 21.81 |
| ATOM | 4545 | CA  | VAL | B | 285 | 52.238 | 15.089 | 65.112 | 1.000 | 29.13 |
| ATOM | 4546 | CB  | VAL | B | 285 | 53.540 | 14.760 | 65.869 | 1.000 | 29.57 |
| ATOM | 4547 | CG1 | VAL | B | 285 | 53.834 | 15.855 | 66.888 | 1.000 | 24.27 |
| ATOM | 4548 | CG2 | VAL | B | 285 | 53.448 | 13.399 | 66.536 | 1.000 | 22.96 |
| ATOM | 4549 | C   | VAL | B | 285 | 51.105 | 15.309 | 66.112 | 1.000 | 27.63 |
| ATOM | 4550 | O   | VAL | B | 285 | 50.869 | 16.442 | 66.513 | 1.000 | 21.60 |
| ATOM | 4551 | N   | HIS | B | 286 | 50.396 | 14.271 | 66.516 | 1.000 | 32.06 |
| ATOM | 4552 | CA  | HIS | B | 286 | 49.336 | 14.195 | 67.498 | 1.000 | 25.21 |
| ATOM | 4553 | CB  | HIS | B | 286 | 49.885 | 14.551 | 68.892 | 1.000 | 28.70 |
| ATOM | 4554 | CG  | HIS | B | 286 | 51.021 | 13.664 | 69.305 | 1.000 | 32.98 |
| ATOM | 4555 | ND1 | HIS | B | 286 | 51.067 | 12.319 | 69.031 | 1.000 | 39.17 |
| ATOM | 4556 | CE1 | HIS | B | 286 | 52.186 | 11.799 | 69.506 | 1.000 | 36.14 |
| ATOM | 4557 | NE2 | HIS | B | 286 | 52.871 | 12.769 | 70.082 | 1.000 | 30.56 |
| ATOM | 4558 | CD2 | HIS | B | 286 | 52.169 | 13.944 | 69.969 | 1.000 | 33.55 |
| ATOM | 4559 | C   | HIS | B | 286 | 48.127 | 15.077 | 67.218 | 1.000 | 30.46 |
| ATOM | 4560 | O   | HIS | B | 286 | 47.387 | 15.403 | 68.154 | 1.000 | 40.44 |
| ATOM | 4561 | N   | MET | B | 287 | 47.881 | 15.467 | 65.973 | 1.000 | 22.86 |
| ATOM | 4562 | CA  | MET | B | 287 | 46.691 | 16.259 | 65.664 | 1.000 | 22.17 |
| ATOM | 4563 | CB  | MET | B | 287 | 46.756 | 16.854 | 64.270 | 1.000 | 18.80 |
| ATOM | 4564 | CG  | MET | B | 287 | 47.775 | 17.949 | 64.042 | 1.000 | 29.11 |
| ATOM | 4565 | SD  | MET | B | 287 | 47.516 | 19.438 | 65.055 | 1.000 | 32.43 |
| ATOM | 4566 | CE  | MET | B | 287 | 48.661 | 19.026 | 66.372 | 1.000 | 13.54 |
| ATOM | 4567 | C   | MET | B | 287 | 45.457 | 15.368 | 65.848 | 1.000 | 29.49 |
| ATOM | 4568 | O   | MET | B | 287 | 45.182 | 14.511 | 65.013 | 1.000 | 22.99 |
| ATOM | 4569 | N   | VAL | B | 288 | 44.774 | 15.611 | 66.952 | 1.000 | 34.12 |
| ATOM | 4570 | CA  | VAL | B | 288 | 43.740 | 14.820 | 67.589 | 1.000 | 28.81 |
| ATOM | 4571 | CB  | VAL | B | 288 | 42.560 | 14.478 | 66.675 | 1.000 | 27.58 |
| ATOM | 4572 | CG1 | VAL | B | 288 | 41.636 | 13.502 | 67.385 | 1.000 | 26.91 |
| ATOM | 4573 | CG2 | VAL | B | 288 | 41.797 | 15.726 | 66.275 | 1.000 | 19.05 |
| ATOM | 4574 | C   | VAL | B | 288 | 44.390 | 13.535 | 68.093 | 1.000 | 30.95 |
| ATOM | 4575 | O   | VAL | B | 288 | 44.556 | 12.583 | 67.334 | 1.000 | 40.72 |

**FIGURE 94**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4576 | N   | GLN | B | 289 | 44.783 | 13.526 | 69.362 | 1.000 | 42.21 |
| ATOM | 4577 | CA  | GLN | B | 289 | 45.728 | 12.504 | 69.827 | 1.000 | 40.64 |
| ATOM | 4578 | CB  | GLN | B | 289 | 46.907 | 13.254 | 70.450 | 1.000 | 38.74 |
| ATOM | 4579 | CG  | GLN | B | 289 | 47.311 | 12.901 | 71.865 | 1.000 | 38.30 |
| ATOM | 4580 | CD  | GLN | B | 289 | 48.223 | 13.989 | 72.413 | 1.000 | 37.90 |
| ATOM | 4581 | OE1 | GLN | B | 289 | 47.738 | 15.038 | 72.837 | 1.000 | 34.96 |
| ATOM | 4582 | NE2 | GLN | B | 289 | 49.525 | 13.736 | 72.392 | 1.000 | 42.59 |
| ATOM | 4583 | C   | GLN | B | 289 | 45.156 | 11.454 | 70.756 | 1.000 | 35.16 |
| ATOM | 4584 | O   | GLN | B | 289 | 45.899 | 10.560 | 71.181 | 1.000 | 34.51 |
| ATOM | 4585 | N   | THR | B | 290 | 43.869 | 11.469 | 71.086 | 1.000 | 27.99 |
| ATOM | 4586 | CA  | THR | B | 290 | 43.294 | 10.342 | 71.819 | 1.000 | 34.56 |
| ATOM | 4587 | CB  | THR | B | 290 | 42.922 | 10.643 | 73.277 | 1.000 | 36.69 |
| ATOM | 4588 | OG1 | THR | B | 290 | 41.958 | 11.699 | 73.369 | 1.000 | 39.54 |
| ATOM | 4589 | CG2 | THR | B | 290 | 44.140 | 11.134 | 74.049 | 1.000 | 28.24 |
| ATOM | 4590 | C   | THR | B | 290 | 42.053 | 9.858  | 71.067 | 1.000 | 45.19 |
| ATOM | 4591 | O   | THR | B | 290 | 41.423 | 10.630 | 70.344 | 1.000 | 37.85 |
| ATOM | 4592 | N   | GLU | B | 291 | 41.708 | 8.583  | 71.228 | 1.000 | 40.04 |
| ATOM | 4593 | CA  | GLU | B | 291 | 40.514 | 8.060  | 70.569 | 1.000 | 31.40 |
| ATOM | 4594 | CB  | GLU | B | 291 | 40.426 | 6.549  | 70.769 | 1.000 | 33.20 |
| ATOM | 4595 | CG  | GLU | B | 291 | 38.992 | 6.033  | 70.734 | 1.000 | 54.35 |
| ATOM | 4596 | CD  | GLU | B | 291 | 38.936 | 4.515  | 70.792 | 1.000 | 61.38 |
| ATOM | 4597 | OE1 | GLU | B | 291 | 37.831 | 3.978  | 71.011 | 1.000 | 56.63 |
| ATOM | 4598 | OE2 | GLU | B | 291 | 40.009 | 3.898  | 70.610 | 1.000 | 65.55 |
| ATOM | 4599 | C   | GLU | B | 291 | 39.274 | 8.756  | 71.108 | 1.000 | 27.13 |
| ATOM | 4600 | O   | GLU | B | 291 | 38.289 | 9.026  | 70.424 | 1.000 | 39.02 |
| ATOM | 4601 | N   | CYS | B | 292 | 39.330 | 9.074  | 72.393 | 1.000 | 30.92 |
| ATOM | 4602 | CA  | CYS | B | 292 | 38.290 | 9.823  | 73.085 | 1.000 | 28.64 |
| ATOM | 4603 | CB  | CYS | B | 292 | 38.815 | 10.131 | 74.493 | 1.000 | 36.66 |
| ATOM | 4604 | SG  | CYS | B | 292 | 37.722 | 11.163 | 75.490 | 1.000 | 55.37 |
| ATOM | 4605 | C   | CYS | B | 292 | 37.903 | 11.103 | 72.351 | 1.000 | 31.79 |
| ATOM | 4606 | O   | CYS | B | 292 | 36.723 | 11.332 | 72.070 | 1.000 | 36.92 |
| ATOM | 4607 | N   | GLN | B | 293 | 38.892 | 11.940 | 72.039 | 1.000 | 33.19 |
| ATOM | 4608 | CA  | GLN | B | 293 | 38.724 | 13.169 | 71.267 | 1.000 | 28.60 |
| ATOM | 4609 | CB  | GLN | B | 293 | 40.056 | 13.880 | 71.039 | 1.000 | 27.95 |
| ATOM | 4610 | CG  | GLN | B | 293 | 40.532 | 14.744 | 72.194 | 1.000 | 27.18 |
| ATOM | 4611 | CD  | GLN | B | 293 | 42.023 | 15.015 | 72.172 | 1.000 | 33.21 |
| ATOM | 4612 | OE1 | GLN | B | 293 | 42.730 | 14.694 | 71.211 | 1.000 | 26.74 |
| ATOM | 4613 | NE2 | GLN | B | 293 | 42.533 | 15.611 | 73.245 | 1.000 | 24.69 |
| ATOM | 4614 | C   | GLN | B | 293 | 38.076 | 12.811 | 69.931 | 1.000 | 28.40 |
| ATOM | 4615 | O   | GLN | B | 293 | 37.089 | 13.407 | 69.513 | 1.000 | 41.52 |
| ATOM | 4616 | N   | TYR | B | 294 | 38.647 | 11.795 | 69.281 | 1.000 | 24.64 |
| ATOM | 4617 | CA  | TYR | B | 294 | 38.065 | 11.284 | 68.041 | 1.000 | 29.87 |
| ATOM | 4618 | CB  | TYR | B | 294 | 38.826 | 10.059 | 67.528 | 1.000 | 35.21 |
| ATOM | 4619 | CG  | TYR | B | 294 | 38.549 | 9.719  | 66.079 | 1.000 | 39.63 |
| ATOM | 4620 | CD1 | TYR | B | 294 | 38.696 | 10.672 | 65.081 | 1.000 | 28.61 |
| ATOM | 4621 | CE1 | TYR | B | 294 | 38.451 | 10.386 | 63.754 | 1.000 | 28.44 |
| ATOM | 4622 | CZ  | TYR | B | 294 | 38.047 | 9.119  | 63.401 | 1.000 | 38.28 |
| ATOM | 4623 | OH  | TYR | B | 294 | 37.803 | 8.837  | 62.078 | 1.000 | 41.13 |
| ATOM | 4624 | CE2 | TYR | B | 294 | 37.891 | 8.151  | 64.368 | 1.000 | 40.14 |
| ATOM | 4625 | CD2 | TYR | B | 294 | 38.141 | 8.446  | 65.695 | 1.000 | 38.49 |
| ATOM | 4626 | C   | TYR | B | 294 | 36.603 | 10.923 | 68.261 | 1.000 | 28.62 |
| ATOM | 4627 | O   | TYR | B | 294 | 35.741 | 11.211 | 67.434 | 1.000 | 36.24 |

**FIGURE 95**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4628 | N   | VAL | B | 295 | 36.302 | 10.285 | 69.396 | 1.000 | 34.52 |
| ATOM | 4629 | CA  | VAL | B | 295 | 34.910 | 9.921  | 69.662 | 1.000 | 31.51 |
| ATOM | 4630 | CB  | VAL | B | 295 | 34.752 | 9.065  | 70.932 | 1.000 | 35.21 |
| ATOM | 4631 | CG1 | VAL | B | 295 | 33.272 | 8.911  | 71.238 | 1.000 | 40.28 |
| ATOM | 4632 | CG2 | VAL | B | 295 | 35.432 | 7.720  | 70.755 | 1.000 | 35.85 |
| ATOM | 4633 | C   | VAL | B | 295 | 34.043 | 11.161 | 69.834 | 1.000 | 27.72 |
| ATOM | 4634 | O   | VAL | B | 295 | 32.911 | 11.223 | 69.360 | 1.000 | 36.42 |
| ATOM | 4635 | N   | TYR | B | 296 | 34.613 | 12.139 | 70.527 | 1.000 | 37.43 |
| ATOM | 4636 | CA  | TYR | B | 296 | 33.941 | 13.417 | 70.761 | 1.000 | 36.42 |
| ATOM | 4637 | CB  | TYR | B | 296 | 34.866 | 14.321 | 71.578 | 1.000 | 43.28 |
| ATOM | 4638 | CG  | TYR | B | 296 | 34.259 | 15.599 | 72.102 | 1.000 | 42.68 |
| ATOM | 4639 | CD1 | TYR | B | 296 | 33.533 | 15.620 | 73.285 | 1.000 | 41.40 |
| ATOM | 4640 | CE1 | TYR | B | 296 | 32.979 | 16.794 | 73.765 | 1.000 | 39.34 |
| ATOM | 4641 | CZ  | TYR | B | 296 | 33.146 | 17.964 | 73.062 | 1.000 | 34.82 |
| ATOM | 4642 | OH  | TYR | B | 296 | 32.597 | 19.132 | 73.530 | 1.000 | 27.53 |
| ATOM | 4643 | CE2 | TYR | B | 296 | 33.865 | 17.973 | 71.884 | 1.000 | 41.20 |
| ATOM | 4644 | CD2 | TYR | B | 296 | 34.415 | 16.796 | 71.415 | 1.000 | 43.82 |
| ATOM | 4645 | C   | TYR | B | 296 | 33.527 | 14.083 | 69.458 | 1.000 | 28.58 |
| ATOM | 4646 | O   | TYR | B | 296 | 32.421 | 14.622 | 69.341 | 1.000 | 31.47 |
| ATOM | 4647 | N   | LEU | B | 297 | 34.403 | 14.066 | 68.453 | 1.000 | 30.22 |
| ATOM | 4648 | CA  | LEU | B | 297 | 34.076 | 14.745 | 67.196 | 1.000 | 30.67 |
| ATOM | 4649 | CB  | LEU | B | 297 | 35.195 | 14.583 | 66.180 | 1.000 | 30.58 |
| ATOM | 4650 | CG  | LEU | B | 297 | 36.483 | 15.373 | 66.375 | 1.000 | 32.73 |
| ATOM | 4651 | CD1 | LEU | B | 297 | 37.535 | 14.919 | 65.367 | 1.000 | 29.68 |
| ATOM | 4652 | CD2 | LEU | B | 297 | 36.220 | 16.866 | 66.250 | 1.000 | 27.24 |
| ATOM | 4653 | C   | LEU | B | 297 | 32.782 | 14.187 | 66.605 | 1.000 | 33.83 |
| ATOM | 4654 | O   | LEU | B | 297 | 31.891 | 14.932 | 66.215 | 1.000 | 31.16 |
| ATOM | 4655 | N   | HIS | B | 298 | 32.737 | 12.860 | 66.570 | 1.000 | 41.22 |
| ATOM | 4656 | CA  | HIS | B | 298 | 31.562 | 12.114 | 66.138 | 1.000 | 38.95 |
| ATOM | 4657 | CB  | HIS | B | 298 | 31.818 | 10.612 | 66.255 | 1.000 | 34.71 |
| ATOM | 4658 | CG  | HIS | B | 298 | 32.822 | 10.070 | 65.285 | 1.000 | 34.66 |
| ATOM | 4659 | ND1 | HIS | B | 298 | 34.177 | 10.070 | 65.531 | 1.000 | 40.08 |
| ATOM | 4660 | CE1 | HIS | B | 298 | 34.825 | 9.528  | 64.511 | 1.000 | 38.60 |
| ATOM | 4661 | NE2 | HIS | B | 298 | 33.935 | 9.166  | 63.602 | 1.000 | 36.65 |
| ATOM | 4662 | CD2 | HIS | B | 298 | 32.679 | 9.494  | 64.071 | 1.000 | 35.52 |
| ATOM | 4663 | C   | HIS | B | 298 | 30.340 | 12.523 | 66.951 | 1.000 | 36.47 |
| ATOM | 4664 | O   | HIS | B | 298 | 29.314 | 12.914 | 66.389 | 1.000 | 36.46 |
| ATOM | 4665 | N   | GLN | B | 299 | 30.420 | 12.464 | 68.280 | 1.000 | 33.50 |
| ATOM | 4666 | CA  | GLN | B | 299 | 29.250 | 12.855 | 69.073 | 1.000 | 36.05 |
| ATOM | 4667 | CB  | GLN | B | 299 | 29.525 | 12.674 | 70.563 | 1.000 | 39.72 |
| ATOM | 4668 | CG  | GLN | B | 299 | 30.053 | 11.279 | 70.887 | 1.000 | 48.51 |
| ATOM | 4669 | CD  | GLN | B | 299 | 30.367 | 11.132 | 72.362 | 1.000 | 53.01 |
| ATOM | 4670 | OE1 | GLN | B | 299 | 30.932 | 12.045 | 72.967 | 1.000 | 50.76 |
| ATOM | 4671 | NE2 | GLN | B | 299 | 29.999 | 9.994  | 72.931 | 1.000 | 51.27 |
| ATOM | 4672 | C   | GLN | B | 299 | 28.841 | 14.289 | 68.782 | 1.000 | 38.19 |
| ATOM | 4673 | O   | GLN | B | 299 | 27.660 | 14.644 | 68.781 | 1.000 | 36.44 |
| ATOM | 4674 | N   | CYS | B | 300 | 29.837 | 15.136 | 68.520 | 1.000 | 36.51 |
| ATOM | 4675 | CA  | CYS | B | 300 | 29.496 | 16.519 | 68.201 | 1.000 | 31.01 |
| ATOM | 4676 | CB  | CYS | B | 300 | 30.752 | 17.368 | 68.017 | 1.000 | 32.05 |
| ATOM | 4677 | SG  | CYS | B | 300 | 31.545 | 17.931 | 69.542 | 1.000 | 33.82 |
| ATOM | 4678 | C   | CYS | B | 300 | 28.665 | 16.568 | 66.925 | 1.000 | 30.84 |
| ATOM | 4679 | O   | CYS | B | 300 | 27.706 | 17.327 | 66.828 | 1.000 | 37.19 |

**FIGURE 96**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 4680 | N   | VAL | B | 301 | 29.042 | 15.767 | 65.927 | 1.000 | 30.57 |
| ATOM | 4681 | CA  | VAL | B | 301 | 28.357 | 15.877 | 64.636 | 1.000 | 35.77 |
| ATOM | 4682 | CB  | VAL | B | 301 | 29.131 | 15.124 | 63.542 | 1.000 | 37.54 |
| ATOM | 4683 | CG1 | VAL | B | 301 | 28.252 | 14.886 | 62.327 | 1.000 | 28.37 |
| ATOM | 4684 | CG2 | VAL | B | 301 | 30.380 | 15.915 | 63.165 | 1.000 | 38.14 |
| ATOM | 4685 | C   | VAL | B | 301 | 26.925 | 15.369 | 64.735 | 1.000 | 39.26 |
| ATOM | 4686 | O   | VAL | B | 301 | 25.977 | 16.025 | 64.295 | 1.000 | 52.69 |
| ATOM | 4687 | N   | ARG | B | 302 | 26.736 | 14.201 | 65.327 | 1.000 | 38.31 |
| ATOM | 4688 | CA  | ARG | B | 302 | 25.403 | 13.654 | 65.555 | 1.000 | 45.66 |
| ATOM | 4689 | CB  | ARG | B | 302 | 25.506 | 12.385 | 66.410 | 1.000 | 42.74 |
| ATOM | 4690 | CG  | ARG | B | 302 | 24.268 | 12.102 | 67.240 | 1.000 | 46.88 |
| ATOM | 4691 | CD  | ARG | B | 302 | 24.579 | 11.103 | 68.354 | 1.000 | 45.04 |
| ATOM | 4692 | NE  | ARG | B | 302 | 25.118 | 11.799 | 69.513 | 1.000 | 48.32 |
| ATOM | 4693 | CZ  | ARG | B | 302 | 25.697 | 11.252 | 70.567 | 1.000 | 45.65 |
| ATOM | 4694 | NH1 | ARG | B | 302 | 25.838 | 9.937  | 70.659 | 1.000 | 43.04 |
| ATOM | 4695 | NH2 | ARG | B | 302 | 26.131 | 12.057 | 71.531 | 1.000 | 48.35 |
| ATOM | 4696 | C   | ARG | B | 302 | 24.480 | 14.642 | 66.256 | 1.000 | 54.36 |
| ATOM | 4697 | O   | ARG | B | 302 | 23.339 | 14.882 | 65.856 | 1.000 | 40.59 |
| ATOM | 4698 | N   | ASP | B | 303 | 24.975 | 15.234 | 67.348 | 1.000 | 56.40 |
| ATOM | 4699 | CA  | ASP | B | 303 | 24.142 | 16.171 | 68.100 | 1.000 | 55.70 |
| ATOM | 4700 | CB  | ASP | B | 303 | 24.898 | 16.662 | 69.342 | 1.000 | 57.02 |
| ATOM | 4701 | CG  | ASP | B | 303 | 25.181 | 15.521 | 70.303 | 1.000 | 59.83 |
| ATOM | 4702 | OD1 | ASP | B | 303 | 24.651 | 14.412 | 70.073 | 1.000 | 59.82 |
| ATOM | 4703 | OD2 | ASP | B | 303 | 25.930 | 15.724 | 71.281 | 1.000 | 60.83 |
| ATOM | 4704 | C   | ASP | B | 303 | 23.688 | 17.342 | 67.236 | 1.000 | 50.72 |
| ATOM | 4705 | O   | ASP | B | 303 | 22.538 | 17.775 | 67.357 | 1.000 | 47.41 |
| ATOM | 4706 | N   | VAL | B | 304 | 24.571 | 17.839 | 66.374 | 1.000 | 44.96 |
| ATOM | 4707 | CA  | VAL | B | 304 | 24.268 | 18.980 | 65.512 | 1.000 | 47.93 |
| ATOM | 4708 | CB  | VAL | B | 304 | 25.515 | 19.435 | 64.739 | 1.000 | 46.69 |
| ATOM | 4709 | CG1 | VAL | B | 304 | 25.147 | 20.348 | 63.575 | 1.000 | 43.96 |
| ATOM | 4710 | CG2 | VAL | B | 304 | 26.484 | 20.141 | 65.677 | 1.000 | 44.01 |
| ATOM | 4711 | C   | VAL | B | 304 | 23.137 | 18.626 | 64.546 | 1.000 | 53.73 |
| ATOM | 4712 | O   | VAL | B | 304 | 22.178 | 19.375 | 64.347 | 1.000 | 37.08 |
| ATOM | 4713 | N   | LEU | B | 305 | 23.286 | 17.442 | 63.958 | 1.000 | 51.48 |
| ATOM | 4714 | CA  | LEU | B | 305 | 22.264 | 16.852 | 63.108 | 1.000 | 52.53 |
| ATOM | 4715 | CB  | LEU | B | 305 | 22.789 | 15.569 | 62.455 | 1.000 | 39.00 |
| ATOM | 4716 | CG  | LEU | B | 305 | 24.083 | 15.749 | 61.649 | 1.000 | 37.23 |
| ATOM | 4717 | CD1 | LEU | B | 305 | 24.587 | 14.409 | 61.143 | 1.000 | 51.92 |
| ATOM | 4718 | CD2 | LEU | B | 305 | 23.868 | 16.711 | 60.496 | 1.000 | 36.51 |
| ATOM | 4719 | C   | LEU | B | 305 | 20.979 | 16.583 | 63.901 | 1.000 | 53.75 |
| ATOM | 4720 | O   | LEU | B | 305 | 19.939 | 17.100 | 63.476 | 1.000 | 35.65 |
| ATOM | 4721 | N   | ARG | B | 306 | 21.076 | 15.820 | 64.980 | 1.000 | 57.84 |
| ATOM | 4722 | CA  | ARG | B | 306 | 20.003 | 15.505 | 65.913 | 1.000 | 58.04 |
| ATOM | 4723 | CB  | ARG | B | 306 | 20.540 | 15.067 | 67.268 | 1.000 | 54.34 |
| ATOM | 4724 | CG  | ARG | B | 306 | 20.660 | 13.573 | 67.496 | 1.000 | 55.97 |
| ATOM | 4725 | CD  | ARG | B | 306 | 21.035 | 13.272 | 68.943 | 1.000 | 61.19 |
| ATOM | 4726 | NE  | ARG | B | 306 | 21.719 | 11.995 | 69.097 | 1.000 | 68.99 |
| ATOM | 4727 | CZ  | ARG | B | 306 | 21.752 | 11.249 | 70.190 | 1.000 | 74.79 |
| ATOM | 4728 | NH1 | ARG | B | 306 | 21.132 | 11.608 | 71.304 | 1.000 | 69.23 |
| ATOM | 4729 | NH2 | ARG | B | 306 | 22.421 | 10.100 | 70.183 | 1.000 | 80.87 |
| ATOM | 4730 | C   | ARG | B | 306 | 19.118 | 16.738 | 66.111 | 1.000 | 62.20 |
| ATOM | 4731 | O   | ARG | B | 306 | 17.971 | 16.763 | 65.681 | 1.000 | 63.69 |

FIGURE 97

|      |      |     |     |   |     |        |         |        |       |        |
|------|------|-----|-----|---|-----|--------|---------|--------|-------|--------|
| ATOM | 4732 | N   | ALA | B | 307 | 19.734 | 17.737  | 66.728 | 1.000 | 65.49  |
| ATOM | 4733 | CA  | ALA | B | 307 | 19.143 | 19.057  | 66.891 | 1.000 | 64.51  |
| ATOM | 4734 | CB  | ALA | B | 307 | 20.143 | 19.994  | 67.558 | 1.000 | 51.87  |
| ATOM | 4735 | C   | ALA | B | 307 | 18.680 | 19.605  | 65.548 | 1.000 | 64.66  |
| ATOM | 4736 | O   | ALA | B | 307 | 17.611 | 20.209  | 65.423 | 1.000 | 65.97  |
| ATOM | 4737 | N   | ARG | B | 308 | 19.468 | 19.412  | 64.491 | 1.000 | 61.42  |
| ATOM | 4738 | CA  | ARG | B | 308 | 19.012 | 19.929  | 63.193 | 1.000 | 70.94  |
| ATOM | 4739 | CB  | ARG | B | 308 | 20.088 | 19.697  | 62.137 | 1.000 | 76.27  |
| ATOM | 4740 | CG  | ARG | B | 308 | 19.741 | 20.209  | 60.748 | 1.000 | 86.23  |
| ATOM | 4741 | CD  | ARG | B | 308 | 20.397 | 21.547  | 60.456 | 1.000 | 95.24  |
| ATOM | 4742 | NE  | ARG | B | 308 | 21.821 | 21.417  | 60.163 | 1.000 | 101.38 |
| ATOM | 4743 | CZ  | ARG | B | 308 | 22.786 | 21.666  | 61.049 | 1.000 | 107.77 |
| ATOM | 4744 | NH1 | ARG | B | 308 | 22.485 | 22.054  | 62.288 | 1.000 | 110.29 |
| ATOM | 4745 | NH2 | ARG | B | 308 | 24.056 | 21.519  | 60.695 | 1.000 | 113.92 |
| ATOM | 4746 | C   | ARG | B | 308 | 17.685 | 19.293  | 62.787 | 1.000 | 73.80  |
| ATOM | 4747 | O   | ARG | B | 308 | 16.827 | 19.955  | 62.197 | 1.000 | 73.18  |
| ATOM | 4748 | N   | LYS | B | 309 | 17.486 | 18.015  | 63.102 | 1.000 | 73.43  |
| ATOM | 4749 | CA  | LYS | B | 309 | 16.283 | 17.286  | 62.718 | 1.000 | 76.77  |
| ATOM | 4750 | CB  | LYS | B | 309 | 16.472 | 15.788  | 62.979 | 1.000 | 79.31  |
| ATOM | 4751 | CG  | LYS | B | 309 | 17.591 | 15.149  | 62.164 | 1.000 | 80.69  |
| ATOM | 4752 | CD  | LYS | B | 309 | 17.436 | 13.637  | 62.104 | 1.000 | 82.88  |
| ATOM | 4753 | CE  | LYS | B | 309 | 18.186 | 13.050  | 60.925 | 1.000 | 82.69  |
| ATOM | 4754 | NZ  | LYS | B | 309 | 19.523 | 12.501  | 61.319 | 1.000 | 75.87  |
| ATOM | 4755 | C   | LYS | B | 309 | 15.033 | 17.778  | 63.442 | 1.000 | 74.89  |
| ATOM | 4756 | O   | LYS | B | 309 | 14.006 | 18.014  | 62.802 | 1.000 | 70.03  |
| ATOM | 4757 | N   | LEU | B | 310 | 15.106 | 17.915  | 64.760 | 1.000 | 66.81  |
| ATOM | 4758 | CA  | LEU | B | 310 | 13.993 | 18.391  | 65.566 | 1.000 | 57.56  |
| ATOM | 4759 | CB  | LEU | B | 310 | 14.439 | 18.679  | 67.003 | 1.000 | 58.43  |
| ATOM | 4760 | CG  | LEU | B | 310 | 14.439 | 17.504  | 67.980 | 1.000 | 59.58  |
| ATOM | 4761 | CD1 | LEU | B | 310 | 15.451 | 17.728  | 69.090 | 1.000 | 37.85  |
| ATOM | 4762 | CD2 | LEU | B | 310 | 13.055 | 17.278  | 68.570 | 1.000 | 65.92  |
| ATOM | 4763 | C   | LEU | B | 310 | 13.371 | 19.657  | 64.978 | 1.000 | 57.95  |
| ATOM | 4764 | O   | LEU | B | 310 | 12.371 | 20.157  | 65.507 | 1.000 | 56.97  |
| ATOM | 4765 | O1  | HOH | W | 1   | -3.530 | -2.470  | 27.550 | 1.000 | 17.96  |
| ATOM | 4766 | O1  | HOH | W | 2   | 60.077 | 26.796  | 63.038 | 1.000 | 15.33  |
| ATOM | 4767 | O1  | HOH | W | 3   | 55.045 | 17.613  | 63.918 | 1.000 | 20.66  |
| ATOM | 4768 | O1  | HOH | W | 4   | 10.035 | -6.431  | 48.617 | 1.000 | 19.03  |
| ATOM | 4769 | O1  | HOH | W | 5   | -2.541 | 7.405   | 22.573 | 1.000 | 24.15  |
| ATOM | 4770 | O1  | HOH | W | 6   | -1.465 | 3.010   | 37.742 | 1.000 | 20.37  |
| ATOM | 4771 | O1  | HOH | W | 7   | 1.064  | 6.887   | 29.228 | 1.000 | 21.37  |
| ATOM | 4772 | O1  | HOH | W | 8   | 12.797 | -10.463 | 28.170 | 1.000 | 21.33  |
| ATOM | 4773 | O1  | HOH | W | 9   | 44.023 | 30.928  | 82.230 | 1.000 | 23.35  |
| ATOM | 4774 | O1  | HOH | W | 10  | 15.262 | -6.127  | 25.706 | 1.000 | 20.03  |
| ATOM | 4775 | O1  | HOH | W | 11  | 41.135 | 13.077  | 75.806 | 1.000 | 24.83  |
| ATOM | 4776 | O1  | HOH | W | 12  | 44.160 | 35.266  | 61.596 | 1.000 | 21.20  |
| ATOM | 4777 | O1  | HOH | W | 13  | -2.293 | 13.135  | 27.030 | 1.000 | 29.16  |
| ATOM | 4778 | O1  | HOH | W | 14  | -1.152 | -4.851  | 36.331 | 1.000 | 18.92  |
| ATOM | 4779 | O1  | HOH | W | 15  | 12.494 | -9.297  | 20.888 | 1.000 | 32.44  |
| ATOM | 4780 | O1  | HOH | W | 16  | 10.561 | -4.413  | 17.800 | 1.000 | 27.50  |
| ATOM | 4781 | O1  | HOH | W | 17  | 12.953 | -1.978  | 15.793 | 1.000 | 23.51  |
| ATOM | 4782 | O1  | HOH | W | 18  | 54.169 | 29.526  | 70.613 | 1.000 | 20.32  |
| ATOM | 4783 | O1  | HOH | W | 19  | 13.709 | 11.416  | 42.827 | 1.000 | 18.88  |

FIGURE 98

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Three Dimensional Coordinates of HPTPbeta

|      |      |    |     |   |    |         |         |        |       |       |
|------|------|----|-----|---|----|---------|---------|--------|-------|-------|
| ATOM | 4784 | O1 | HOH | W | 20 | 55.731  | 28.213  | 80.604 | 1.000 | 26.83 |
| ATOM | 4785 | O1 | HOH | W | 21 | 4.760   | 11.444  | 27.886 | 1.000 | 20.66 |
| ATOM | 4786 | O1 | HOH | W | 22 | 56.913  | 29.110  | 71.387 | 1.000 | 17.72 |
| ATOM | 4787 | O1 | HOH | W | 23 | 18.440  | -8.145  | 47.574 | 1.000 | 28.67 |
| ATOM | 4788 | O1 | HOH | W | 24 | 51.613  | 13.126  | 62.266 | 1.000 | 25.40 |
| ATOM | 4789 | O1 | HOH | W | 25 | 56.785  | 21.500  | 72.666 | 1.000 | 22.09 |
| ATOM | 4790 | O1 | HOH | W | 26 | 46.913  | 32.045  | 55.417 | 1.000 | 36.86 |
| ATOM | 4791 | O1 | HOH | W | 27 | 10.490  | -7.264  | 21.479 | 1.000 | 24.68 |
| ATOM | 4792 | O1 | HOH | W | 28 | -4.811  | -5.788  | 33.716 | 1.000 | 23.37 |
| ATOM | 4793 | O1 | HOH | W | 29 | 58.662  | 11.046  | 62.178 | 1.000 | 28.32 |
| ATOM | 4794 | O1 | HOH | W | 30 | 40.935  | 36.024  | 75.388 | 1.000 | 36.78 |
| ATOM | 4795 | O1 | HOH | W | 31 | 56.949  | 30.099  | 57.221 | 1.000 | 20.47 |
| ATOM | 4796 | O1 | HOH | W | 32 | 45.404  | 15.934  | 74.179 | 1.000 | 31.95 |
| ATOM | 4797 | O1 | HOH | W | 33 | -6.695  | -5.778  | 43.032 | 1.000 | 31.77 |
| ATOM | 4798 | O1 | HOH | W | 34 | 46.397  | 21.045  | 76.403 | 1.000 | 35.06 |
| ATOM | 4799 | O1 | HOH | W | 35 | 60.957  | 30.231  | 69.118 | 1.000 | 21.63 |
| ATOM | 4800 | O1 | HOH | W | 36 | -3.350  | -17.246 | 31.808 | 1.000 | 41.60 |
| ATOM | 4801 | O1 | HOH | W | 37 | 55.555  | 12.895  | 71.190 | 1.000 | 29.48 |
| ATOM | 4802 | O1 | HOH | W | 38 | 1.468   | -5.097  | 35.986 | 1.000 | 22.35 |
| ATOM | 4803 | O1 | HOH | W | 39 | 15.156  | -9.650  | 27.646 | 1.000 | 20.92 |
| ATOM | 4804 | O1 | HOH | W | 40 | 38.773  | 25.200  | 57.849 | 1.000 | 23.39 |
| ATOM | 4805 | O1 | HOH | W | 41 | 10.348  | 17.067  | 32.030 | 1.000 | 41.46 |
| ATOM | 4806 | O1 | HOH | W | 42 | 1.648   | -14.559 | 44.147 | 1.000 | 28.83 |
| ATOM | 4807 | O1 | HOH | W | 43 | 61.596  | 20.901  | 62.903 | 1.000 | 28.38 |
| ATOM | 4808 | O1 | HOH | W | 44 | 14.144  | -11.298 | 42.153 | 1.000 | 36.30 |
| ATOM | 4809 | O1 | HOH | W | 45 | 59.647  | 17.031  | 57.868 | 1.000 | 23.78 |
| ATOM | 4810 | O1 | HOH | W | 46 | 53.695  | 23.952  | 54.917 | 1.000 | 39.83 |
| ATOM | 4811 | O1 | HOH | W | 47 | 27.056  | 31.327  | 66.272 | 1.000 | 55.85 |
| ATOM | 4812 | O1 | HOH | W | 48 | 37.053  | 41.920  | 74.032 | 1.000 | 46.26 |
| ATOM | 4813 | O1 | HOH | W | 49 | -2.397  | 0.653   | 20.483 | 1.000 | 37.18 |
| ATOM | 4814 | O1 | HOH | W | 50 | 41.473  | 15.741  | 75.531 | 1.000 | 43.52 |
| ATOM | 4815 | O1 | HOH | W | 51 | -2.370  | -15.863 | 33.885 | 1.000 | 30.41 |
| ATOM | 4816 | O1 | HOH | W | 52 | -12.538 | 6.131   | 27.682 | 1.000 | 29.52 |
| ATOM | 4817 | O1 | HOH | W | 53 | 53.221  | 16.883  | 55.102 | 1.000 | 33.14 |
| ATOM | 4818 | O1 | HOH | W | 54 | 14.966  | -8.503  | 24.747 | 1.000 | 25.12 |
| ATOM | 4819 | O1 | HOH | W | 55 | 8.494   | -4.831  | 50.889 | 1.000 | 30.18 |
| ATOM | 4820 | O1 | HOH | W | 56 | 24.585  | -9.942  | 22.611 | 1.000 | 54.01 |
| ATOM | 4821 | O1 | HOH | W | 57 | 18.441  | -20.771 | 46.004 | 1.000 | 39.24 |
| ATOM | 4822 | O1 | HOH | W | 58 | 51.873  | 22.607  | 56.086 | 1.000 | 29.82 |
| ATOM | 4823 | O1 | HOH | W | 59 | 1.396   | -6.152  | 18.909 | 1.000 | 47.00 |
| ATOM | 4824 | O1 | HOH | W | 60 | 44.607  | 38.534  | 81.740 | 1.000 | 40.03 |
| ATOM | 4825 | O1 | HOH | W | 61 | 18.322  | -0.373  | 24.933 | 1.000 | 28.92 |
| ATOM | 4826 | O1 | HOH | W | 62 | 39.406  | 39.382  | 64.024 | 1.000 | 36.75 |
| ATOM | 4827 | O1 | HOH | W | 63 | 71.786  | 42.646  | 67.354 | 1.000 | 38.18 |
| ATOM | 4828 | O1 | HOH | W | 64 | 41.387  | 20.207  | 52.496 | 1.000 | 61.66 |
| ATOM | 4829 | O1 | HOH | W | 65 | 58.599  | 39.944  | 69.257 | 1.000 | 22.54 |
| ATOM | 4830 | O1 | HOH | W | 66 | 7.902   | 0.663   | 20.612 | 1.000 | 25.67 |
| ATOM | 4831 | O1 | HOH | W | 67 | 49.818  | 23.739  | 54.522 | 1.000 | 26.64 |
| ATOM | 4832 | O1 | HOH | W | 68 | 0.323   | -5.848  | 22.222 | 1.000 | 21.16 |
| ATOM | 4833 | O1 | HOH | W | 69 | 8.339   | -2.798  | 16.062 | 1.000 | 35.15 |
| ATOM | 4834 | O1 | HOH | W | 70 | 10.628  | -6.726  | 18.494 | 1.000 | 23.48 |
| ATOM | 4835 | O1 | HOH | W | 71 | 34.368  | 9.766   | 58.834 | 1.000 | 46.05 |

**FIGURE 99**

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Three Dimensional Coordinates of HPTPbeta

|      |      |    |     |   |     |         |         |        |       |       |
|------|------|----|-----|---|-----|---------|---------|--------|-------|-------|
| ATOM | 4836 | O1 | HOH | W | 72  | 0.104   | -9.966  | 24.934 | 1.000 | 31.25 |
| ATOM | 4837 | O1 | HOH | W | 73  | -3.205  | -3.781  | 34.722 | 1.000 | 24.34 |
| ATOM | 4838 | O1 | HOH | W | 74  | 40.443  | 25.217  | 78.384 | 1.000 | 21.19 |
| ATOM | 4839 | O1 | HOH | W | 75  | 60.161  | 17.919  | 77.858 | 1.000 | 43.49 |
| ATOM | 4840 | O1 | HOH | W | 76  | 57.383  | 25.403  | 56.423 | 1.000 | 28.69 |
| ATOM | 4841 | O1 | HOH | W | 77  | -0.918  | -4.290  | 45.708 | 1.000 | 23.94 |
| ATOM | 4842 | O1 | HOH | W | 78  | 39.671  | 29.793  | 57.818 | 1.000 | 28.43 |
| ATOM | 4843 | O1 | HOH | W | 79  | -0.151  | -0.962  | 21.277 | 1.000 | 31.95 |
| ATOM | 4844 | O1 | HOH | W | 80  | 7.936   | -8.337  | 20.044 | 1.000 | 31.62 |
| ATOM | 4845 | O1 | HOH | W | 81  | 41.764  | 30.809  | 59.091 | 1.000 | 32.37 |
| ATOM | 4846 | O1 | HOH | W | 82  | 16.518  | -9.547  | 23.062 | 1.000 | 37.01 |
| ATOM | 4847 | O1 | HOH | W | 83  | 30.713  | 30.994  | 77.311 | 1.000 | 33.53 |
| ATOM | 4848 | O1 | HOH | W | 84  | 28.454  | -2.369  | 72.054 | 1.000 | 47.39 |
| ATOM | 4849 | O1 | HOH | W | 85  | -5.917  | -8.292  | 22.002 | 1.000 | 37.83 |
| ATOM | 4850 | O1 | HOH | W | 86  | 7.580   | -10.565 | 21.487 | 1.000 | 31.50 |
| ATOM | 4851 | O1 | HOH | W | 87  | 13.747  | 8.631   | 42.204 | 1.000 | 29.91 |
| ATOM | 4852 | O1 | HOH | W | 88  | 34.378  | 8.211   | 61.163 | 1.000 | 35.02 |
| ATOM | 4853 | O1 | HOH | W | 89  | 55.698  | 21.340  | 61.326 | 1.000 | 34.48 |
| ATOM | 4854 | O1 | HOH | W | 90  | -0.448  | -6.040  | 47.787 | 1.000 | 38.54 |
| ATOM | 4855 | O1 | HOH | W | 91  | -0.537  | -4.018  | 20.186 | 1.000 | 52.78 |
| ATOM | 4856 | O1 | HOH | W | 92  | 58.171  | 28.185  | 55.468 | 1.000 | 35.33 |
| ATOM | 4857 | O1 | HOH | W | 93  | -1.835  | -17.836 | 29.482 | 1.000 | 43.68 |
| ATOM | 4858 | O1 | HOH | W | 94  | 19.387  | -17.439 | 48.725 | 1.000 | 53.98 |
| ATOM | 4859 | O1 | HOH | W | 95  | 60.252  | 41.304  | 67.862 | 1.000 | 40.39 |
| ATOM | 4860 | O1 | HOH | W | 96  | 33.297  | 25.666  | 61.866 | 1.000 | 30.40 |
| ATOM | 4861 | O1 | HOH | W | 97  | -0.856  | -8.441  | 21.984 | 1.000 | 40.05 |
| ATOM | 4862 | O1 | HOH | W | 98  | 1.309   | 3.127   | 26.649 | 1.000 | 32.55 |
| ATOM | 4863 | O1 | HOH | W | 99  | -1.694  | -18.493 | 42.845 | 1.000 | 43.76 |
| ATOM | 4864 | O1 | HOH | W | 100 | 24.060  | -6.419  | 45.384 | 1.000 | 40.45 |
| ATOM | 4865 | O1 | HOH | W | 101 | -16.201 | 0.201   | 30.012 | 1.000 | 60.21 |
| ATOM | 4866 | O1 | HOH | W | 102 | 26.465  | -8.482  | 43.564 | 1.000 | 39.40 |
| ATOM | 4867 | O1 | HOH | W | 103 | 26.382  | -4.680  | 30.946 | 1.000 | 37.07 |
| ATOM | 4868 | O1 | HOH | W | 104 | 14.152  | -0.770  | 45.187 | 1.000 | 31.90 |
| ATOM | 4869 | O1 | HOH | W | 105 | 45.353  | 7.442   | 65.377 | 1.000 | 41.13 |
| ATOM | 4870 | O1 | HOH | W | 106 | 61.574  | 29.765  | 78.858 | 1.000 | 30.33 |
| ATOM | 4871 | O1 | HOH | W | 107 | 7.240   | 13.732  | 33.506 | 1.000 | 51.68 |
| ATOM | 4872 | O1 | HOH | W | 108 | 63.827  | 31.328  | 67.142 | 1.000 | 34.68 |
| ATOM | 4873 | O1 | HOH | W | 109 | 27.765  | 8.197   | 72.253 | 1.000 | 40.60 |
| ATOM | 4874 | O1 | HOH | W | 110 | 26.746  | 31.022  | 63.432 | 1.000 | 78.25 |
| ATOM | 4875 | O1 | HOH | W | 111 | 5.779   | 12.491  | 31.119 | 1.000 | 40.18 |
| ATOM | 4876 | O1 | HOH | W | 112 | 0.254   | 17.249  | 30.260 | 1.000 | 37.62 |
| ATOM | 4877 | O1 | HOH | W | 113 | 12.595  | 10.239  | 20.359 | 1.000 | 35.26 |
| ATOM | 4878 | O1 | HOH | W | 114 | -12.231 | 8.847   | 27.346 | 1.000 | 34.71 |
| ATOM | 4879 | O1 | HOH | W | 115 | 6.080   | 14.549  | 28.922 | 1.000 | 38.97 |
| ATOM | 4880 | O1 | HOH | W | 116 | 42.291  | 33.445  | 57.940 | 1.000 | 22.41 |
| ATOM | 4881 | O1 | HOH | W | 117 | 59.009  | 28.099  | 70.085 | 1.000 | 25.15 |
| ATOM | 4882 | O1 | HOH | W | 118 | 21.222  | 2.455   | 47.444 | 1.000 | 48.38 |
| ATOM | 4883 | O1 | HOH | W | 119 | 15.608  | -16.455 | 31.001 | 1.000 | 42.95 |
| ATOM | 4884 | O1 | HOH | W | 120 | -0.125  | 11.690  | 36.476 | 1.000 | 30.48 |
| ATOM | 4885 | O1 | HOH | W | 121 | 1.726   | 11.454  | 38.848 | 1.000 | 32.74 |
| ATOM | 4886 | O1 | HOH | W | 122 | 28.290  | -0.445  | 30.933 | 1.000 | 38.16 |
| ATOM | 4887 | O1 | HOH | W | 123 | 6.212   | -24.378 | 36.045 | 1.000 | 44.15 |

**FIGURE 100**



|      |      |    |           |         |         |        |       |        |
|------|------|----|-----------|---------|---------|--------|-------|--------|
| ATOM | 4888 | O1 | HOH W 124 | 1.177   | -29.065 | 27.544 | 1.000 | 45.02  |
| ATOM | 4889 | O1 | HOH W 125 | 56.979  | 34.259  | 60.005 | 1.000 | 48.14  |
| ATOM | 4890 | O1 | HOH W 126 | 58.730  | 33.237  | 57.099 | 1.000 | 45.63  |
| ATOM | 4891 | O1 | HOH W 127 | 15.046  | 11.322  | 20.955 | 1.000 | 40.69  |
| ATOM | 4892 | O1 | HOH W 128 | 17.468  | -4.910  | 24.971 | 1.000 | 27.77  |
| ATOM | 4893 | O1 | HOH W 129 | -7.587  | -7.450  | 31.742 | 1.000 | 42.13  |
| ATOM | 4894 | O1 | HOH W 130 | 62.587  | 23.632  | 57.526 | 1.000 | 35.90  |
| ATOM | 4895 | O1 | HOH W 131 | -1.756  | 3.962   | 17.316 | 1.000 | 54.25  |
| ATOM | 4896 | O1 | HOH W 132 | -7.965  | -8.197  | 36.101 | 1.000 | 44.77  |
| ATOM | 4897 | O1 | HOH W 133 | 24.522  | -12.151 | 40.839 | 1.000 | 47.60  |
| ATOM | 4898 | O1 | HOH W 134 | 41.871  | 34.231  | 60.791 | 1.000 | 28.90  |
| ATOM | 4899 | O1 | HOH W 135 | 0.084   | 1.514   | 45.812 | 1.000 | 36.86  |
| ATOM | 4900 | O1 | HOH W 136 | -8.408  | 3.637   | 36.615 | 1.000 | 38.14  |
| ATOM | 4901 | O1 | HOH W 137 | 40.900  | 41.156  | 64.403 | 1.000 | 36.63  |
| ATOM | 4902 | O1 | HOH W 138 | -11.020 | -17.691 | 22.512 | 1.000 | 75.97  |
| ATOM | 4903 | O1 | HOH W 139 | 7.850   | 3.732   | 42.421 | 1.000 | 36.40  |
| ATOM | 4904 | O1 | HOH W 140 | 26.443  | -10.866 | 28.599 | 1.000 | 51.16  |
| ATOM | 4905 | O1 | HOH W 141 | 23.109  | 4.111   | 20.091 | 1.000 | 51.94  |
| ATOM | 4906 | O1 | HOH W 142 | 38.297  | 16.036  | 84.787 | 1.000 | 45.01  |
| ATOM | 4907 | O1 | HOH W 143 | 21.913  | 17.019  | 28.707 | 1.000 | 43.32  |
| ATOM | 4908 | O1 | HOH W 144 | 59.964  | 41.572  | 65.028 | 1.000 | 58.77  |
| ATOM | 4909 | O1 | HOH W 145 | 46.873  | 21.994  | 79.174 | 1.000 | 40.67  |
| ATOM | 4910 | O1 | HOH W 146 | 19.058  | -16.861 | 40.797 | 1.000 | 48.41  |
| ATOM | 4911 | O1 | HOH W 147 | 50.103  | 11.202  | 73.004 | 1.000 | 41.20  |
| ATOM | 4912 | O1 | HOH W 148 | -3.801  | 9.680   | 21.040 | 1.000 | 40.17  |
| ATOM | 4913 | O1 | HOH W 149 | 0.486   | 8.561   | 18.811 | 1.000 | 40.75  |
| ATOM | 4914 | O1 | HOH W 150 | 19.935  | 8.387   | 60.381 | 1.000 | 53.72  |
| ATOM | 4915 | O1 | HOH W 151 | 23.477  | -0.731  | 29.783 | 1.000 | 32.64  |
| ATOM | 4916 | O1 | HOH W 152 | 43.876  | 43.513  | 55.758 | 1.000 | 69.30  |
| ATOM | 4917 | O1 | HOH W 153 | -5.161  | 3.525   | 27.477 | 1.000 | 32.16  |
| ATOM | 4918 | O1 | HOH W 154 | 41.525  | 16.199  | 52.939 | 1.000 | 81.81  |
| ATOM | 4919 | O1 | HOH W 155 | -4.928  | -12.335 | 20.354 | 1.000 | 61.63  |
| ATOM | 4920 | O1 | HOH W 156 | 13.058  | 0.354   | 47.602 | 1.000 | 30.77  |
| ATOM | 4921 | O1 | HOH W 157 | 43.059  | 17.423  | 76.789 | 1.000 | 45.11  |
| ATOM | 4922 | O1 | HOH W 158 | 62.494  | 11.714  | 59.113 | 1.000 | 108.46 |
| ATOM | 4923 | O1 | HOH W 159 | 48.631  | 10.662  | 67.791 | 1.000 | 38.71  |
| ATOM | 4924 | O1 | HOH W 160 | 36.309  | 22.824  | 83.433 | 1.000 | 53.78  |
| ATOM | 4925 | O1 | HOH W 161 | 34.255  | 41.203  | 81.271 | 1.000 | 58.61  |
| ATOM | 4926 | O1 | HOH W 162 | 41.197  | 23.937  | 80.959 | 1.000 | 34.06  |
| ATOM | 4927 | O1 | HOH W 163 | 41.828  | 13.385  | 50.732 | 1.000 | 77.14  |
| ATOM | 4928 | O1 | HOH W 164 | 31.641  | 33.672  | 55.019 | 1.000 | 59.40  |
| ATOM | 4929 | O1 | HOH W 165 | 15.868  | 14.555  | 66.209 | 1.000 | 65.90  |
| ATOM | 4930 | O1 | HOH W 166 | 57.742  | 42.116  | 78.337 | 1.000 | 65.62  |
| ATOM | 4931 | O1 | HOH W 167 | 4.617   | -25.082 | 27.972 | 1.000 | 47.28  |
| ATOM | 4932 | O1 | HOH W 168 | 2.787   | 17.721  | 23.213 | 1.000 | 98.79  |
| ATOM | 4933 | O1 | HOH W 169 | 59.715  | 23.680  | 80.391 | 1.000 | 59.77  |
| ATOM | 4934 | O1 | HOH W 170 | 37.169  | 14.176  | 35.477 | 1.000 | 57.67  |
| ATOM | 4935 | O1 | HOH W 171 | 15.841  | -25.349 | 41.958 | 1.000 | 68.09  |
| ATOM | 4936 | O1 | HOH W 172 | 69.007  | 25.633  | 74.020 | 1.000 | 68.84  |
| ATOM | 4937 | O1 | HOH W 173 | 63.270  | 32.699  | 57.782 | 1.000 | 41.40  |
| ATOM | 4938 | O1 | HOH W 174 | 38.069  | 44.790  | 79.133 | 1.000 | 74.12  |
| ATOM | 4939 | O1 | HOH W 175 | 74.296  | 43.345  | 65.746 | 1.000 | 58.77  |

**FIGURE 101**

|      |      |    |           |         |         |        |       |        |
|------|------|----|-----------|---------|---------|--------|-------|--------|
| ATOM | 4940 | O1 | HOH W 176 | 29.671  | 29.752  | 62.465 | 1.000 | 48.75  |
| ATOM | 4941 | O1 | HOH W 177 | 27.349  | 16.661  | 41.834 | 1.000 | 64.12  |
| ATOM | 4942 | O1 | HOH W 178 | 68.864  | 18.200  | 64.263 | 1.000 | 44.37  |
| ATOM | 4943 | O1 | HOH W 179 | 51.540  | 25.428  | 52.448 | 1.000 | 52.06  |
| ATOM | 4944 | O1 | HOH W 180 | 28.343  | -0.494  | 74.952 | 1.000 | 90.20  |
| ATOM | 4945 | O1 | HOH W 181 | -12.972 | -6.360  | 31.919 | 1.000 | 61.07  |
| ATOM | 4946 | O1 | HOH W 182 | 29.627  | 16.979  | 37.935 | 1.000 | 63.71  |
| ATOM | 4947 | O1 | HOH W 183 | 30.147  | -2.678  | 28.953 | 1.000 | 52.59  |
| ATOM | 4948 | O1 | HOH W 184 | 55.934  | 13.116  | 53.037 | 1.000 | 49.11  |
| ATOM | 4949 | O1 | HOH W 185 | -4.863  | -11.799 | 39.588 | 1.000 | 42.83  |
| ATOM | 4950 | O1 | HOH W 186 | 52.756  | 41.765  | 58.587 | 1.000 | 57.97  |
| ATOM | 4951 | O1 | HOH W 187 | 27.188  | -2.332  | 27.244 | 1.000 | 43.06  |
| ATOM | 4952 | O1 | HOH W 188 | 30.473  | 7.380   | 75.791 | 1.000 | 81.10  |
| ATOM | 4953 | O1 | HOH W 189 | -7.908  | -19.633 | 34.839 | 1.000 | 59.42  |
| ATOM | 4954 | O1 | HOH W 190 | 28.733  | 14.583  | 42.278 | 1.000 | 54.80  |
| ATOM | 4955 | O1 | HOH W 191 | -13.906 | -5.879  | 34.683 | 1.000 | 54.42  |
| ATOM | 4956 | O1 | HOH W 192 | 60.646  | 30.561  | 54.430 | 1.000 | 103.36 |
| ATOM | 4957 | O1 | HOH W 193 | 35.855  | 14.670  | 80.980 | 1.000 | 52.28  |
| ATOM | 4958 | O1 | HOH W 194 | 19.267  | -7.719  | 50.684 | 1.000 | 99.38  |
| ATOM | 4959 | O1 | HOH W 195 | 17.702  | -14.597 | 31.579 | 1.000 | 48.72  |
| ATOM | 4960 | O1 | HOH W 196 | 25.127  | 1.357   | 21.179 | 1.000 | 86.89  |
| ATOM | 4961 | O1 | HOH W 197 | 7.136   | 23.308  | 30.331 | 1.000 | 67.50  |
| ATOM | 4962 | O1 | HOH W 198 | 66.979  | 28.356  | 73.926 | 1.000 | 73.15  |
| ATOM | 4963 | O1 | HOH W 199 | 58.649  | 27.550  | 81.422 | 1.000 | 51.44  |
| ATOM | 4964 | O1 | HOH W 200 | 26.717  | 16.527  | 75.237 | 1.000 | 49.85  |
| ATOM | 4965 | O1 | HOH W 201 | 50.540  | 18.935  | 78.454 | 1.000 | 49.28  |

END

**FIGURE 102**

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Three Dimensional Coordinates of HPTPbeta

|        |        |        |        |       |       |        |        |                   |
|--------|--------|--------|--------|-------|-------|--------|--------|-------------------|
| CRYST1 | 62.186 | 71.797 | 70.448 | 90.00 | 93.56 | 90.00  |        |                   |
| ATOM   | 1      | N      | THR    | A     | 20    | 13.220 | 15.647 | 19.635 1.00 51.11 |
| ATOM   | 2      | CA     | THR    | A     | 20    | 14.046 | 16.499 | 20.485 1.00 49.11 |
| ATOM   | 3      | CB     | THR    | A     | 20    | 13.219 | 17.270 | 21.525 1.00 56.84 |
| ATOM   | 4      | OG1    | THR    | A     | 20    | 11.822 | 17.025 | 21.318 1.00 82.00 |
| ATOM   | 5      | CG2    | THR    | A     | 20    | 13.411 | 18.771 | 21.351 1.00 62.78 |
| ATOM   | 6      | C      | THR    | A     | 20    | 15.126 | 15.682 | 21.189 1.00 47.28 |
| ATOM   | 7      | O      | THR    | A     | 20    | 14.920 | 14.601 | 21.731 1.00 36.27 |
| ATOM   | 8      | N      | SER    | A     | 21    | 16.332 | 16.238 | 21.145 1.00 41.80 |
| ATOM   | 9      | CA     | SER    | A     | 21    | 17.525 | 15.585 | 21.640 1.00 38.45 |
| ATOM   | 10     | CB     | SER    | A     | 21    | 18.027 | 14.556 | 20.623 1.00 50.01 |
| ATOM   | 11     | OG     | SER    | A     | 21    | 18.114 | 15.125 | 19.328 1.00 57.39 |
| ATOM   | 12     | C      | SER    | A     | 21    | 18.628 | 16.597 | 21.924 1.00 40.97 |
| ATOM   | 13     | O      | SER    | A     | 21    | 18.818 | 17.552 | 21.172 1.00 54.77 |
| ATOM   | 14     | N      | CYS    | A     | 22    | 19.351 | 16.377 | 23.013 1.00 38.55 |
| ATOM   | 15     | CA     | CYS    | A     | 22    | 20.465 | 17.251 | 23.365 1.00 41.82 |
| ATOM   | 16     | CB     | CYS    | A     | 22    | 20.194 | 17.972 | 24.677 1.00 49.07 |
| ATOM   | 17     | SG     | CYS    | A     | 22    | 21.184 | 19.448 | 24.992 1.00157.91 |
| ATOM   | 18     | C      | CYS    | A     | 22    | 21.737 | 16.416 | 23.433 1.00 40.34 |
| ATOM   | 19     | O      | CYS    | A     | 22    | 22.215 | 16.085 | 24.518 1.00 48.60 |
| ATOM   | 20     | N      | PRO    | A     | 23    | 22.270 | 16.062 | 22.271 1.00 32.99 |
| ATOM   | 21     | CA     | PRO    | A     | 23    | 23.464 | 15.210 | 22.261 1.00 38.72 |
| ATOM   | 22     | CB     | PRO    | A     | 23    | 23.710 | 14.926 | 20.790 1.00 42.84 |
| ATOM   | 23     | CG     | PRO    | A     | 23    | 22.474 | 15.348 | 20.073 1.00 43.60 |
| ATOM   | 24     | CD     | PRO    | A     | 23    | 21.836 | 16.415 | 20.914 1.00 38.82 |
| ATOM   | 25     | C      | PRO    | A     | 23    | 24.615 | 15.995 | 22.881 1.00 48.13 |
| ATOM   | 26     | O      | PRO    | A     | 23    | 24.711 | 17.211 | 22.701 1.00 47.03 |
| ATOM   | 27     | N      | ILE    | A     | 24    | 25.460 | 15.298 | 23.625 1.00 44.75 |
| ATOM   | 28     | CA     | ILE    | A     | 24    | 26.566 | 15.975 | 24.297 1.00 44.40 |
| ATOM   | 29     | CB     | ILE    | A     | 24    | 26.272 | 16.206 | 25.788 1.00 42.81 |
| ATOM   | 30     | CG1    | ILE    | A     | 24    | 25.075 | 17.122 | 26.057 1.00 46.37 |
| ATOM   | 31     | CD1    | ILE    | A     | 24    | 24.076 | 16.565 | 27.047 1.00 66.22 |
| ATOM   | 32     | CG2    | ILE    | A     | 24    | 27.512 | 16.726 | 26.502 1.00 39.08 |
| ATOM   | 33     | C      | ILE    | A     | 24    | 27.832 | 15.154 | 24.125 1.00 40.83 |
| ATOM   | 34     | O      | ILE    | A     | 24    | 27.907 | 13.977 | 24.460 1.00 37.86 |
| ATOM   | 35     | N      | LYS    | A     | 25    | 28.852 | 15.794 | 23.569 1.00 44.53 |
| ATOM   | 36     | CA     | LYS    | A     | 25    | 30.123 | 15.105 | 23.390 1.00 43.13 |
| ATOM   | 37     | CB     | LYS    | A     | 25    | 31.053 | 15.966 | 22.534 1.00 53.45 |
| ATOM   | 38     | CG     | LYS    | A     | 25    | 30.471 | 16.274 | 21.159 1.00 54.09 |
| ATOM   | 39     | CD     | LYS    | A     | 25    | 31.401 | 15.816 | 20.047 1.00 53.48 |
| ATOM   | 40     | CE     | LYS    | A     | 25    | 30.749 | 14.744 | 19.184 1.00 52.46 |
| ATOM   | 41     | NZ     | LYS    | A     | 25    | 31.611 | 13.534 | 19.051 1.00 56.82 |
| ATOM   | 42     | C      | LYS    | A     | 25    | 30.742 | 14.777 | 24.743 1.00 35.84 |
| ATOM   | 43     | O      | LYS    | A     | 25    | 30.676 | 15.549 | 25.699 1.00 35.11 |
| ATOM   | 44     | N      | ILE    | A     | 26    | 31.342 | 13.599 | 24.805 1.00 30.07 |
| ATOM   | 45     | CA     | ILE    | A     | 26    | 31.956 | 13.072 | 26.009 1.00 44.79 |
| ATOM   | 46     | CB     | ILE    | A     | 26    | 32.828 | 11.842 | 25.666 1.00 53.22 |
| ATOM   | 47     | CG1    | ILE    | A     | 26    | 32.077 | 10.710 | 24.967 1.00 52.52 |
| ATOM   | 48     | CD1    | ILE    | A     | 26    | 30.646 | 10.520 | 25.409 1.00 30.26 |
| ATOM   | 49     | CG2    | ILE    | A     | 26    | 33.540 | 11.331 | 26.909 1.00 64.21 |
| ATOM   | 50     | C      | ILE    | A     | 26    | 32.827 | 14.089 | 26.738 1.00 48.16 |
| ATOM   | 51     | O      | ILE    | A     | 26    | 32.683 | 14.275 | 27.948 1.00 50.00 |

**FIGURE 103**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 52  | N   | ASN | A | 27 | 33.731 | 14.732 | 26.005 | 1.00 | 46.06 |
| ATOM | 53  | CA  | ASN | A | 27 | 34.745 | 15.593 | 26.605 | 1.00 | 48.63 |
| ATOM | 54  | CB  | ASN | A | 27 | 35.900 | 15.802 | 25.627 | 1.00 | 60.83 |
| ATOM | 55  | CG  | ASN | A | 27 | 35.840 | 16.989 | 24.701 | 1.00 | 62.73 |
| ATOM | 56  | OD1 | ASN | A | 27 | 34.812 | 17.621 | 24.451 | 1.00 | 61.11 |
| ATOM | 57  | ND2 | ASN | A | 27 | 37.003 | 17.330 | 24.140 | 1.00 | 50.07 |
| ATOM | 58  | C   | ASN | A | 27 | 34.158 | 16.914 | 27.075 | 1.00 | 49.04 |
| ATOM | 59  | O   | ASN | A | 27 | 34.843 | 17.726 | 27.705 | 1.00 | 47.37 |
| ATOM | 60  | N   | GLN | A | 28 | 32.878 | 17.141 | 26.778 | 1.00 | 46.15 |
| ATOM | 61  | CA  | GLN | A | 28 | 32.271 | 18.381 | 27.266 | 1.00 | 49.97 |
| ATOM | 62  | CB  | GLN | A | 28 | 31.655 | 19.163 | 26.101 | 1.00 | 56.77 |
| ATOM | 63  | CG  | GLN | A | 28 | 32.595 | 19.346 | 24.918 | 1.00 | 66.10 |
| ATOM | 64  | CD  | GLN | A | 28 | 32.102 | 20.390 | 23.934 | 1.00 | 71.73 |
| ATOM | 65  | OE1 | GLN | A | 28 | 31.403 | 21.326 | 24.320 | 1.00 | 72.33 |
| ATOM | 66  | NE2 | GLN | A | 28 | 32.453 | 20.244 | 22.661 | 1.00 | 76.09 |
| ATOM | 67  | C   | GLN | A | 28 | 31.227 | 18.109 | 28.337 | 1.00 | 40.82 |
| ATOM | 68  | O   | GLN | A | 28 | 30.634 | 19.039 | 28.895 | 1.00 | 38.64 |
| ATOM | 69  | N   | PHE | A | 29 | 30.965 | 16.838 | 28.647 | 1.00 | 40.55 |
| ATOM | 70  | CA  | PHE | A | 29 | 29.821 | 16.576 | 29.522 | 1.00 | 33.60 |
| ATOM | 71  | CB  | PHE | A | 29 | 29.591 | 15.064 | 29.660 | 1.00 | 39.21 |
| ATOM | 72  | CG  | PHE | A | 29 | 28.380 | 14.777 | 30.544 | 1.00 | 32.38 |
| ATOM | 73  | CD1 | PHE | A | 29 | 27.109 | 14.865 | 30.005 | 1.00 | 33.31 |
| ATOM | 74  | CE1 | PHE | A | 29 | 25.985 | 14.624 | 30.772 | 1.00 | 33.30 |
| ATOM | 75  | CZ  | PHE | A | 29 | 26.136 | 14.282 | 32.103 | 1.00 | 38.62 |
| ATOM | 76  | CE2 | PHE | A | 29 | 27.402 | 14.192 | 32.648 | 1.00 | 37.08 |
| ATOM | 77  | CD2 | PHE | A | 29 | 28.520 | 14.426 | 31.874 | 1.00 | 28.51 |
| ATOM | 78  | C   | PHE | A | 29 | 29.981 | 17.210 | 30.898 | 1.00 | 25.63 |
| ATOM | 79  | O   | PHE | A | 29 | 29.074 | 17.856 | 31.430 | 1.00 | 40.09 |
| ATOM | 80  | N   | GLU | A | 30 | 31.161 | 17.013 | 31.469 | 1.00 | 36.23 |
| ATOM | 81  | CA  | GLU | A | 30 | 31.510 | 17.549 | 32.778 | 1.00 | 43.91 |
| ATOM | 82  | CB  | GLU | A | 30 | 33.004 | 17.328 | 33.045 | 1.00 | 55.32 |
| ATOM | 83  | CG  | GLU | A | 30 | 33.738 | 16.650 | 31.903 | 1.00 | 66.32 |
| ATOM | 84  | CD  | GLU | A | 30 | 33.492 | 15.158 | 31.798 | 1.00 | 75.29 |
| ATOM | 85  | OE1 | GLU | A | 30 | 33.517 | 14.458 | 32.833 | 1.00 | 81.66 |
| ATOM | 86  | OE2 | GLU | A | 30 | 33.270 | 14.685 | 30.659 | 1.00 | 78.35 |
| ATOM | 87  | C   | GLU | A | 30 | 31.153 | 19.024 | 32.895 | 1.00 | 33.72 |
| ATOM | 88  | O   | GLU | A | 30 | 30.421 | 19.428 | 33.800 | 1.00 | 34.69 |
| ATOM | 89  | N   | GLY | A | 31 | 31.659 | 19.845 | 31.973 | 1.00 | 36.69 |
| ATOM | 90  | CA  | GLY | A | 31 | 31.407 | 21.279 | 32.045 | 1.00 | 29.29 |
| ATOM | 91  | C   | GLY | A | 31 | 29.939 | 21.581 | 31.824 | 1.00 | 40.96 |
| ATOM | 92  | O   | GLY | A | 31 | 29.333 | 22.407 | 32.512 | 1.00 | 37.93 |
| ATOM | 93  | N   | HIS | A | 32 | 29.401 | 20.867 | 30.835 | 1.00 | 51.96 |
| ATOM | 94  | CA  | HIS | A | 32 | 27.980 | 20.958 | 30.502 | 1.00 | 44.37 |
| ATOM | 95  | CB  | HIS | A | 32 | 27.638 | 19.919 | 29.443 | 1.00 | 58.95 |
| ATOM | 96  | CG  | HIS | A | 32 | 26.265 | 19.339 | 29.512 | 1.00 | 69.53 |
| ATOM | 97  | ND1 | HIS | A | 32 | 25.190 | 19.878 | 28.841 | 1.00 | 71.46 |
| ATOM | 98  | CE1 | HIS | A | 32 | 24.109 | 19.159 | 29.083 | 1.00 | 73.05 |
| ATOM | 99  | NE2 | HIS | A | 32 | 24.441 | 18.167 | 29.890 | 1.00 | 73.89 |
| ATOM | 100 | CD2 | HIS | A | 32 | 25.783 | 18.259 | 30.170 | 1.00 | 73.95 |
| ATOM | 101 | C   | HIS | A | 32 | 27.176 | 20.784 | 31.777 | 1.00 | 40.30 |
| ATOM | 102 | O   | HIS | A | 32 | 26.380 | 21.635 | 32.177 | 1.00 | 35.23 |
| ATOM | 103 | N   | PHE | A | 33 | 27.414 | 19.655 | 32.448 | 1.00 | 37.93 |

**FIGURE 104**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 104 | CA  | PHE | A | 33 | 26.660 | 19.416 | 33.684 | 1.00 | 35.86 |
| ATOM | 105 | CB  | PHE | A | 33 | 27.026 | 18.033 | 34.233 | 1.00 | 30.87 |
| ATOM | 106 | CG  | PHE | A | 33 | 26.146 | 17.593 | 35.390 | 1.00 | 31.86 |
| ATOM | 107 | CD1 | PHE | A | 33 | 24.793 | 17.870 | 35.387 | 1.00 | 30.87 |
| ATOM | 108 | CE1 | PHE | A | 33 | 23.998 | 17.487 | 36.449 | 1.00 | 39.07 |
| ATOM | 109 | CZ  | PHE | A | 33 | 24.556 | 16.815 | 37.521 | 1.00 | 40.71 |
| ATOM | 110 | CE2 | PHE | A | 33 | 25.911 | 16.528 | 37.534 | 1.00 | 33.73 |
| ATOM | 111 | CD2 | PHE | A | 33 | 26.694 | 16.911 | 36.464 | 1.00 | 32.41 |
| ATOM | 112 | C   | PHE | A | 33 | 26.888 | 20.531 | 34.694 | 1.00 | 33.77 |
| ATOM | 113 | O   | PHE | A | 33 | 25.952 | 20.961 | 35.381 | 1.00 | 36.95 |
| ATOM | 114 | N   | MET | A | 34 | 28.109 | 21.054 | 34.812 | 1.00 | 40.28 |
| ATOM | 115 | CA  | MET | A | 34 | 28.365 | 22.163 | 35.733 | 1.00 | 36.53 |
| ATOM | 116 | CB  | MET | A | 34 | 29.840 | 22.550 | 35.715 | 1.00 | 37.70 |
| ATOM | 117 | CG  | MET | A | 34 | 30.725 | 21.619 | 36.533 | 1.00 | 44.64 |
| ATOM | 118 | SD  | MET | A | 34 | 32.467 | 21.981 | 36.237 | 1.00 | 57.03 |
| ATOM | 119 | CE  | MET | A | 34 | 32.639 | 23.515 | 37.150 | 1.00 | 38.10 |
| ATOM | 120 | C   | MET | A | 34 | 27.538 | 23.393 | 35.382 | 1.00 | 32.51 |
| ATOM | 121 | O   | MET | A | 34 | 26.955 | 24.065 | 36.235 | 1.00 | 52.72 |
| ATOM | 122 | N   | LYS | A | 35 | 27.508 | 23.672 | 34.081 | 1.00 | 35.94 |
| ATOM | 123 | CA  | LYS | A | 35 | 26.695 | 24.776 | 33.583 | 1.00 | 42.22 |
| ATOM | 124 | CB  | LYS | A | 35 | 26.769 | 24.818 | 32.059 | 1.00 | 53.72 |
| ATOM | 125 | CG  | LYS | A | 35 | 27.490 | 26.026 | 31.488 | 1.00 | 64.13 |
| ATOM | 126 | CD  | LYS | A | 35 | 26.830 | 26.522 | 30.211 | 1.00 | 73.45 |
| ATOM | 127 | CE  | LYS | A | 35 | 25.799 | 27.603 | 30.481 | 1.00 | 79.66 |
| ATOM | 128 | NZ  | LYS | A | 35 | 25.397 | 28.334 | 29.244 | 1.00 | 65.59 |
| ATOM | 129 | C   | LYS | A | 35 | 25.261 | 24.606 | 34.072 | 1.00 | 42.89 |
| ATOM | 130 | O   | LYS | A | 35 | 24.679 | 25.467 | 34.733 | 1.00 | 40.73 |
| ATOM | 131 | N   | LEU | A | 36 | 24.707 | 23.441 | 33.733 | 1.00 | 35.38 |
| ATOM | 132 | CA  | LEU | A | 36 | 23.356 | 23.091 | 34.131 | 1.00 | 26.66 |
| ATOM | 133 | CB  | LEU | A | 36 | 23.027 | 21.631 | 33.793 | 1.00 | 34.71 |
| ATOM | 134 | CG  | LEU | A | 36 | 22.556 | 21.329 | 32.373 | 1.00 | 35.84 |
| ATOM | 135 | CD1 | LEU | A | 36 | 23.700 | 21.485 | 31.388 | 1.00 | 40.98 |
| ATOM | 136 | CD2 | LEU | A | 36 | 21.974 | 19.922 | 32.277 | 1.00 | 32.82 |
| ATOM | 137 | C   | LEU | A | 36 | 23.172 | 23.283 | 35.629 | 1.00 | 24.20 |
| ATOM | 138 | O   | LEU | A | 36 | 22.123 | 23.748 | 36.062 | 1.00 | 28.20 |
| ATOM | 139 | N   | GLN | A | 37 | 24.207 | 22.901 | 36.378 | 1.00 | 25.36 |
| ATOM | 140 | CA  | GLN | A | 37 | 24.143 | 22.963 | 37.831 | 1.00 | 31.18 |
| ATOM | 141 | CB  | GLN | A | 37 | 25.189 | 22.007 | 38.420 | 1.00 | 38.07 |
| ATOM | 142 | CG  | GLN | A | 37 | 24.588 | 20.611 | 38.573 | 1.00 | 46.59 |
| ATOM | 143 | CD  | GLN | A | 37 | 25.546 | 19.648 | 39.244 | 1.00 | 51.11 |
| ATOM | 144 | OE1 | GLN | A | 37 | 26.637 | 19.410 | 38.728 | 1.00 | 44.66 |
| ATOM | 145 | NE2 | GLN | A | 37 | 25.114 | 19.115 | 40.378 | 1.00 | 36.68 |
| ATOM | 146 | C   | GLN | A | 37 | 24.337 | 24.373 | 38.379 | 1.00 | 40.44 |
| ATOM | 147 | O   | GLN | A | 37 | 23.814 | 24.666 | 39.455 | 1.00 | 35.38 |
| ATOM | 148 | N   | ALA | A | 38 | 25.050 | 25.199 | 37.630 | 1.00 | 45.31 |
| ATOM | 149 | CA  | ALA | A | 38 | 25.238 | 26.608 | 37.933 | 1.00 | 58.11 |
| ATOM | 150 | CB  | ALA | A | 38 | 25.738 | 27.359 | 36.705 | 1.00 | 66.03 |
| ATOM | 151 | C   | ALA | A | 38 | 23.953 | 27.264 | 38.431 | 1.00 | 66.10 |
| ATOM | 152 | O   | ALA | A | 38 | 22.853 | 26.812 | 38.114 | 1.00 | 78.27 |
| ATOM | 153 | N   | ASP | A | 39 | 24.121 | 28.331 | 39.199 | 1.00 | 68.10 |
| ATOM | 154 | CA  | ASP | A | 39 | 23.041 | 29.104 | 39.794 | 1.00 | 71.28 |
| ATOM | 155 | CB  | ASP | A | 39 | 22.423 | 30.060 | 38.774 | 1.00 | 77.06 |

**FIGURE 105**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |        |
|------|-----|-----|-----|---|----|--------|--------|--------|------|--------|
| ATOM | 156 | CG  | ASP | A | 39 | 23.365 | 30.405 | 37.638 | 1.00 | 86.83  |
| ATOM | 157 | OD1 | ASP | A | 39 | 23.544 | 29.551 | 36.742 | 1.00 | 105.52 |
| ATOM | 158 | OD2 | ASP | A | 39 | 23.932 | 31.516 | 37.639 | 1.00 | 105.04 |
| ATOM | 159 | C   | ASP | A | 39 | 21.969 | 28.188 | 40.383 | 1.00 | 69.59  |
| ATOM | 160 | O   | ASP | A | 39 | 20.770 | 28.436 | 40.271 | 1.00 | 51.64  |
| ATOM | 161 | N   | SER | A | 40 | 22.436 | 27.116 | 41.014 | 1.00 | 72.47  |
| ATOM | 162 | CA  | SER | A | 40 | 21.569 | 26.129 | 41.639 | 1.00 | 73.99  |
| ATOM | 163 | CB  | SER | A | 40 | 20.695 | 26.792 | 42.708 | 1.00 | 78.30  |
| ATOM | 164 | OG  | SER | A | 40 | 20.340 | 25.862 | 43.718 | 1.00 | 96.66  |
| ATOM | 165 | C   | SER | A | 40 | 20.698 | 25.414 | 40.612 | 1.00 | 69.44  |
| ATOM | 166 | O   | SER | A | 40 | 19.473 | 25.380 | 40.738 | 1.00 | 68.61  |
| ATOM | 167 | N   | ASN | A | 41 | 21.324 | 24.836 | 39.588 | 1.00 | 67.73  |
| ATOM | 168 | CA  | ASN | A | 41 | 20.564 | 24.038 | 38.628 | 1.00 | 64.81  |
| ATOM | 169 | CB  | ASN | A | 41 | 19.846 | 22.901 | 39.367 | 1.00 | 61.79  |
| ATOM | 170 | CG  | ASN | A | 41 | 20.795 | 21.929 | 40.031 | 1.00 | 61.73  |
| ATOM | 171 | OD1 | ASN | A | 41 | 22.000 | 21.958 | 39.789 | 1.00 | 69.43  |
| ATOM | 172 | ND2 | ASN | A | 41 | 20.260 | 21.055 | 40.876 | 1.00 | 77.55  |
| ATOM | 173 | C   | ASN | A | 41 | 19.542 | 24.870 | 37.871 | 1.00 | 61.80  |
| ATOM | 174 | O   | ASN | A | 41 | 18.448 | 24.397 | 37.545 | 1.00 | 46.20  |
| ATOM | 175 | N   | TYR | A | 42 | 19.871 | 26.131 | 37.586 | 1.00 | 55.50  |
| ATOM | 176 | CA  | TYR | A | 42 | 18.879 | 26.965 | 36.907 | 1.00 | 53.77  |
| ATOM | 177 | CB  | TYR | A | 42 | 19.293 | 28.437 | 36.963 | 1.00 | 58.34  |
| ATOM | 178 | CG  | TYR | A | 42 | 18.328 | 29.359 | 36.248 | 1.00 | 57.25  |
| ATOM | 179 | CD1 | TYR | A | 42 | 17.106 | 29.704 | 36.812 | 1.00 | 53.13  |
| ATOM | 180 | CE1 | TYR | A | 42 | 16.237 | 30.547 | 36.143 | 1.00 | 55.57  |
| ATOM | 181 | CZ  | TYR | A | 42 | 16.586 | 31.048 | 34.908 | 1.00 | 57.51  |
| ATOM | 182 | OH  | TYR | A | 42 | 15.728 | 31.888 | 34.236 | 1.00 | 77.05  |
| ATOM | 183 | CE2 | TYR | A | 42 | 17.792 | 30.720 | 34.327 | 1.00 | 53.44  |
| ATOM | 184 | CD2 | TYR | A | 42 | 18.652 | 29.878 | 35.001 | 1.00 | 54.42  |
| ATOM | 185 | C   | TYR | A | 42 | 18.676 | 26.523 | 35.463 | 1.00 | 46.65  |
| ATOM | 186 | O   | TYR | A | 42 | 17.565 | 26.523 | 34.925 | 1.00 | 42.26  |
| ATOM | 187 | N   | LEU | A | 43 | 19.772 | 26.135 | 34.813 | 1.00 | 33.69  |
| ATOM | 188 | CA  | LEU | A | 43 | 19.638 | 25.715 | 33.419 | 1.00 | 35.76  |
| ATOM | 189 | CB  | LEU | A | 43 | 20.980 | 25.835 | 32.706 | 1.00 | 39.54  |
| ATOM | 190 | CG  | LEU | A | 43 | 21.238 | 27.199 | 32.047 | 1.00 | 40.56  |
| ATOM | 191 | CD1 | LEU | A | 43 | 20.408 | 28.282 | 32.714 | 1.00 | 40.30  |
| ATOM | 192 | CD2 | LEU | A | 43 | 22.709 | 27.555 | 32.093 | 1.00 | 29.81  |
| ATOM | 193 | C   | LEU | A | 43 | 19.077 | 24.300 | 33.348 | 1.00 | 48.21  |
| ATOM | 194 | O   | LEU | A | 43 | 18.421 | 23.937 | 32.371 | 1.00 | 40.48  |
| ATOM | 195 | N   | LEU | A | 44 | 19.326 | 23.509 | 34.394 | 1.00 | 46.35  |
| ATOM | 196 | CA  | LEU | A | 44 | 18.762 | 22.160 | 34.438 | 1.00 | 44.23  |
| ATOM | 197 | CB  | LEU | A | 44 | 19.440 | 21.300 | 35.503 | 1.00 | 45.17  |
| ATOM | 198 | CG  | LEU | A | 44 | 19.102 | 19.805 | 35.499 | 1.00 | 45.62  |
| ATOM | 199 | CD1 | LEU | A | 44 | 20.365 | 18.965 | 35.586 | 1.00 | 31.11  |
| ATOM | 200 | CD2 | LEU | A | 44 | 18.148 | 19.475 | 36.638 | 1.00 | 39.34  |
| ATOM | 201 | C   | LEU | A | 44 | 17.257 | 22.238 | 34.682 | 1.00 | 40.48  |
| ATOM | 202 | O   | LEU | A | 44 | 16.490 | 21.546 | 34.017 | 1.00 | 46.20  |
| ATOM | 203 | N   | SER | A | 45 | 16.833 | 23.079 | 35.624 | 1.00 | 37.28  |
| ATOM | 204 | CA  | SER | A | 45 | 15.412 | 23.227 | 35.909 | 1.00 | 41.63  |
| ATOM | 205 | CB  | SER | A | 45 | 15.183 | 24.298 | 36.971 | 1.00 | 49.13  |
| ATOM | 206 | OG  | SER | A | 45 | 15.258 | 23.742 | 38.273 | 1.00 | 45.34  |
| ATOM | 207 | C   | SER | A | 45 | 14.644 | 23.557 | 34.635 | 1.00 | 47.28  |

**FIGURE 106**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 208 | O   | SER | A | 45 | 13.532 | 23.071 | 34.420 | 1.00 | 56.54 |
| ATOM | 209 | N   | LYS | A | 46 | 15.239 | 24.377 | 33.775 | 1.00 | 48.99 |
| ATOM | 210 | CA  | LYS | A | 46 | 14.588 | 24.708 | 32.508 | 1.00 | 53.30 |
| ATOM | 211 | CB  | LYS | A | 46 | 15.228 | 25.954 | 31.890 | 1.00 | 59.16 |
| ATOM | 212 | CG  | LYS | A | 46 | 15.006 | 27.210 | 32.725 | 1.00 | 63.86 |
| ATOM | 213 | CD  | LYS | A | 46 | 15.835 | 28.379 | 32.220 | 1.00 | 64.48 |
| ATOM | 214 | CE  | LYS | A | 46 | 15.039 | 29.675 | 32.252 | 1.00 | 64.98 |
| ATOM | 215 | NZ  | LYS | A | 46 | 15.675 | 30.745 | 31.433 | 1.00 | 56.04 |
| ATOM | 216 | C   | LYS | A | 46 | 14.622 | 23.533 | 31.535 | 1.00 | 47.85 |
| ATOM | 217 | O   | LYS | A | 46 | 13.603 | 23.266 | 30.890 | 1.00 | 55.12 |
| ATOM | 218 | N   | GLU | A | 47 | 15.746 | 22.834 | 31.420 | 1.00 | 36.87 |
| ATOM | 219 | CA  | GLU | A | 47 | 15.840 | 21.669 | 30.546 | 1.00 | 45.16 |
| ATOM | 220 | CB  | GLU | A | 47 | 17.247 | 21.060 | 30.588 | 1.00 | 47.65 |
| ATOM | 221 | CG  | GLU | A | 47 | 17.495 | 20.034 | 29.498 | 1.00 | 48.46 |
| ATOM | 222 | CD  | GLU | A | 47 | 18.919 | 19.534 | 29.410 | 1.00 | 55.44 |
| ATOM | 223 | OE1 | GLU | A | 47 | 19.665 | 19.977 | 28.510 | 1.00 | 68.33 |
| ATOM | 224 | OE2 | GLU | A | 47 | 19.316 | 18.675 | 30.229 | 1.00 | 55.44 |
| ATOM | 225 | C   | GLU | A | 47 | 14.799 | 20.615 | 30.918 | 1.00 | 39.97 |
| ATOM | 226 | O   | GLU | A | 47 | 14.010 | 20.178 | 30.080 | 1.00 | 39.03 |
| ATOM | 227 | N   | TYR | A | 48 | 14.770 | 20.191 | 32.177 | 1.00 | 35.97 |
| ATOM | 228 | CA  | TYR | A | 48 | 13.770 | 19.221 | 32.614 | 1.00 | 40.19 |
| ATOM | 229 | CB  | TYR | A | 48 | 13.910 | 18.925 | 34.105 | 1.00 | 35.08 |
| ATOM | 230 | CG  | TYR | A | 48 | 13.004 | 17.856 | 34.671 | 1.00 | 32.74 |
| ATOM | 231 | CD1 | TYR | A | 48 | 13.165 | 16.505 | 34.361 | 1.00 | 28.30 |
| ATOM | 232 | CE1 | TYR | A | 48 | 12.316 | 15.553 | 34.903 | 1.00 | 22.32 |
| ATOM | 233 | CZ  | TYR | A | 48 | 11.301 | 15.922 | 35.753 | 1.00 | 30.86 |
| ATOM | 234 | OH  | TYR | A | 48 | 10.450 | 14.983 | 36.292 | 1.00 | 30.54 |
| ATOM | 235 | CE2 | TYR | A | 48 | 11.115 | 17.253 | 36.080 | 1.00 | 26.20 |
| ATOM | 236 | CD2 | TYR | A | 48 | 11.970 | 18.194 | 35.534 | 1.00 | 28.57 |
| ATOM | 237 | C   | TYR | A | 48 | 12.369 | 19.729 | 32.302 | 1.00 | 49.53 |
| ATOM | 238 | O   | TYR | A | 48 | 11.526 | 19.006 | 31.769 | 1.00 | 51.41 |
| ATOM | 239 | N   | GLU | A | 49 | 12.105 | 20.994 | 32.637 | 1.00 | 46.93 |
| ATOM | 240 | CA  | GLU | A | 49 | 10.772 | 21.536 | 32.378 | 1.00 | 42.89 |
| ATOM | 241 | CB  | GLU | A | 49 | 10.655 | 22.963 | 32.912 | 1.00 | 52.01 |
| ATOM | 242 | CG  | GLU | A | 49 | 9.269  | 23.330 | 33.420 | 1.00 | 65.78 |
| ATOM | 243 | CD  | GLU | A | 49 | 8.788  | 22.347 | 34.472 | 1.00 | 79.04 |
| ATOM | 244 | OE1 | GLU | A | 49 | 9.560  | 22.068 | 35.413 | 1.00 | 96.40 |
| ATOM | 245 | OE2 | GLU | A | 49 | 7.646  | 21.856 | 34.354 | 1.00 | 91.96 |
| ATOM | 246 | C   | GLU | A | 49 | 10.462 | 21.493 | 30.883 | 1.00 | 29.38 |
| ATOM | 247 | O   | GLU | A | 49 | 9.309  | 21.423 | 30.462 | 1.00 | 38.63 |
| ATOM | 248 | N   | GLU | A | 50 | 11.510 | 21.544 | 30.075 | 1.00 | 34.87 |
| ATOM | 249 | CA  | GLU | A | 50 | 11.357 | 21.477 | 28.626 | 1.00 | 46.84 |
| ATOM | 250 | CB  | GLU | A | 50 | 12.745 | 21.550 | 27.998 | 1.00 | 52.28 |
| ATOM | 251 | CG  | GLU | A | 50 | 12.782 | 21.554 | 26.483 | 1.00 | 62.44 |
| ATOM | 252 | CD  | GLU | A | 50 | 13.712 | 22.655 | 25.996 | 1.00 | 72.44 |
| ATOM | 253 | OE1 | GLU | A | 50 | 14.373 | 22.454 | 24.958 | 1.00 | 92.62 |
| ATOM | 254 | OE2 | GLU | A | 50 | 13.753 | 23.697 | 26.686 | 1.00 | 72.72 |
| ATOM | 255 | C   | GLU | A | 50 | 10.644 | 20.199 | 28.208 | 1.00 | 52.30 |
| ATOM | 256 | O   | GLU | A | 50 | 9.964  | 20.114 | 27.186 | 1.00 | 54.37 |
| ATOM | 257 | N   | LEU | A | 51 | 10.816 | 19.164 | 29.028 | 1.00 | 44.46 |
| ATOM | 258 | CA  | LEU | A | 51 | 10.319 | 17.841 | 28.691 | 1.00 | 34.94 |
| ATOM | 259 | CB  | LEU | A | 51 | 11.233 | 16.772 | 29.304 | 1.00 | 24.94 |

**FIGURE 107**

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 260 | CG  | LEU | A | 51 | 12.654 | 16.734 | 28.754 | 1.00 | 21.39 |
| ATOM | 261 | CD1 | LEU | A | 51 | 13.621 | 16.312 | 29.850 | 1.00 | 34.46 |
| ATOM | 262 | CD2 | LEU | A | 51 | 12.731 | 15.811 | 27.550 | 1.00 | 25.27 |
| ATOM | 263 | C   | LEU | A | 51 | 8.912  | 17.588 | 29.202 | 1.00 | 42.88 |
| ATOM | 264 | O   | LEU | A | 51 | 8.350  | 16.541 | 28.883 | 1.00 | 29.33 |
| ATOM | 265 | N   | LYS | A | 52 | 8.399  | 18.530 | 29.983 | 1.00 | 44.99 |
| ATOM | 266 | CA  | LYS | A | 52 | 7.115  | 18.337 | 30.643 | 1.00 | 49.66 |
| ATOM | 267 | CB  | LYS | A | 52 | 6.789  | 19.557 | 31.513 | 1.00 | 57.53 |
| ATOM | 268 | CG  | LYS | A | 52 | 6.095  | 20.683 | 30.765 | 1.00 | 69.23 |
| ATOM | 269 | CD  | LYS | A | 52 | 6.543  | 22.048 | 31.263 | 1.00 | 75.40 |
| ATOM | 270 | CE  | LYS | A | 52 | 5.563  | 23.135 | 30.850 | 1.00 | 81.49 |
| ATOM | 271 | NZ  | LYS | A | 52 | 4.161  | 22.796 | 31.229 | 1.00 | 87.53 |
| ATOM | 272 | C   | LYS | A | 52 | 5.973  | 18.083 | 29.671 | 1.00 | 38.67 |
| ATOM | 273 | O   | LYS | A | 52 | 5.052  | 17.334 | 29.988 | 1.00 | 35.81 |
| ATOM | 274 | N   | ASP | A | 53 | 5.984  | 18.692 | 28.489 | 1.00 | 36.11 |
| ATOM | 275 | CA  | ASP | A | 53 | 4.829  | 18.567 | 27.605 | 1.00 | 40.07 |
| ATOM | 276 | CB  | ASP | A | 53 | 4.529  | 19.928 | 26.954 | 1.00 | 49.22 |
| ATOM | 277 | CG  | ASP | A | 53 | 4.334  | 21.018 | 27.995 | 1.00 | 54.49 |
| ATOM | 278 | OD1 | ASP | A | 53 | 5.153  | 21.961 | 28.039 | 1.00 | 73.06 |
| ATOM | 279 | OD2 | ASP | A | 53 | 3.367  | 20.942 | 28.782 | 1.00 | 35.35 |
| ATOM | 280 | C   | ASP | A | 53 | 5.012  | 17.503 | 26.537 | 1.00 | 32.08 |
| ATOM | 281 | O   | ASP | A | 53 | 4.126  | 17.303 | 25.702 | 1.00 | 27.30 |
| ATOM | 282 | N   | VAL | A | 54 | 6.138  | 16.789 | 26.531 | 1.00 | 23.82 |
| ATOM | 283 | CA  | VAL | A | 54 | 6.275  | 15.745 | 25.515 | 1.00 | 26.43 |
| ATOM | 284 | CB  | VAL | A | 54 | 7.644  | 15.063 | 25.611 | 1.00 | 23.01 |
| ATOM | 285 | CG1 | VAL | A | 54 | 7.804  | 13.986 | 24.545 | 1.00 | 19.26 |
| ATOM | 286 | CG2 | VAL | A | 54 | 8.762  | 16.096 | 25.487 | 1.00 | 34.53 |
| ATOM | 287 | C   | VAL | A | 54 | 5.166  | 14.704 | 25.659 | 1.00 | 26.62 |
| ATOM | 288 | O   | VAL | A | 54 | 4.905  | 14.234 | 26.761 | 1.00 | 17.16 |
| ATOM | 289 | N   | GLY | A | 55 | 4.527  | 14.349 | 24.554 | 1.00 | 21.88 |
| ATOM | 290 | CA  | GLY | A | 55 | 3.558  | 13.282 | 24.475 | 1.00 | 23.39 |
| ATOM | 291 | C   | GLY | A | 55 | 2.195  | 13.617 | 25.024 | 1.00 | 30.22 |
| ATOM | 292 | O   | GLY | A | 55 | 1.314  | 12.758 | 25.104 | 1.00 | 23.51 |
| ATOM | 293 | N   | ARG | A | 56 | 1.989  | 14.875 | 25.405 | 1.00 | 31.50 |
| ATOM | 294 | CA  | ARG | A | 56 | 0.782  | 15.271 | 26.119 | 1.00 | 28.44 |
| ATOM | 295 | CB  | ARG | A | 56 | 0.984  | 16.662 | 26.743 | 1.00 | 36.73 |
| ATOM | 296 | CG  | ARG | A | 56 | 1.082  | 17.789 | 25.719 | 1.00 | 31.99 |
| ATOM | 297 | CD  | ARG | A | 56 | 1.004  | 19.156 | 26.390 | 1.00 | 37.18 |
| ATOM | 298 | NE  | ARG | A | 56 | -0.281 | 19.323 | 27.056 | 1.00 | 43.75 |
| ATOM | 299 | CZ  | ARG | A | 56 | -0.556 | 19.932 | 28.193 | 1.00 | 45.89 |
| ATOM | 300 | NH1 | ARG | A | 56 | 0.380  | 20.516 | 28.923 | 1.00 | 38.18 |
| ATOM | 301 | NH2 | ARG | A | 56 | -1.817 | 19.962 | 28.623 | 1.00 | 39.43 |
| ATOM | 302 | C   | ARG | A | 56 | -0.450 | 15.279 | 25.227 | 1.00 | 29.67 |
| ATOM | 303 | O   | ARG | A | 56 | -1.567 | 15.445 | 25.732 | 1.00 | 27.62 |
| ATOM | 304 | N   | ASN | A | 57 | -0.237 | 15.110 | 23.922 | 1.00 | 26.65 |
| ATOM | 305 | CA  | ASN | A | 57 | -1.345 | 15.090 | 22.982 | 1.00 | 27.28 |
| ATOM | 306 | CB  | ASN | A | 57 | -0.843 | 15.400 | 21.560 | 1.00 | 38.20 |
| ATOM | 307 | CG  | ASN | A | 57 | 0.466  | 14.695 | 21.254 | 1.00 | 54.73 |
| ATOM | 308 | OD1 | ASN | A | 57 | 1.420  | 14.764 | 22.038 | 1.00 | 55.09 |
| ATOM | 309 | ND2 | ASN | A | 57 | 0.530  | 14.011 | 20.113 | 1.00 | 53.28 |
| ATOM | 310 | C   | ASN | A | 57 | -2.063 | 13.752 | 22.942 | 1.00 | 24.18 |
| ATOM | 311 | O   | ASN | A | 57 | -3.083 | 13.668 | 22.252 | 1.00 | 23.88 |

**FIGURE 108**



Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 312 | N   | GLN | A | 58 | -1.579  | 12.719 | 23.623 | 1.00 | 27.84 |
| ATOM | 313 | CA  | GLN | A | 58 | -2.119  | 11.366 | 23.492 | 1.00 | 20.86 |
| ATOM | 314 | CB  | GLN | A | 58 | -0.963  | 10.339 | 23.556 | 1.00 | 16.18 |
| ATOM | 315 | CG  | GLN | A | 58 | -0.004  | 10.576 | 22.386 | 1.00 | 19.18 |
| ATOM | 316 | CD  | GLN | A | 58 | 1.282   | 9.797  | 22.440 | 1.00 | 17.89 |
| ATOM | 317 | OE1 | GLN | A | 58 | 1.430   | 8.818  | 21.702 | 1.00 | 27.40 |
| ATOM | 318 | NE2 | GLN | A | 58 | 2.226   | 10.196 | 23.293 | 1.00 | 22.07 |
| ATOM | 319 | C   | GLN | A | 58 | -3.169  | 11.060 | 24.540 | 1.00 | 24.60 |
| ATOM | 320 | O   | GLN | A | 58 | -3.146  | 11.517 | 25.685 | 1.00 | 28.29 |
| ATOM | 321 | N   | SER | A | 59 | -4.147  | 10.253 | 24.129 | 1.00 | 19.50 |
| ATOM | 322 | CA  | SER | A | 59 | -5.255  | 9.909  | 25.012 | 1.00 | 17.23 |
| ATOM | 323 | CB  | SER | A | 59 | -6.538  | 9.850  | 24.170 | 1.00 | 25.69 |
| ATOM | 324 | OG  | SER | A | 59 | -6.970  | 11.173 | 23.891 | 1.00 | 42.05 |
| ATOM | 325 | C   | SER | A | 59 | -5.039  | 8.570  | 25.710 | 1.00 | 19.80 |
| ATOM | 326 | O   | SER | A | 59 | -4.224  | 7.784  | 25.210 | 1.00 | 16.72 |
| ATOM | 327 | N   | CYS | A | 60 | -5.766  | 8.346  | 26.789 | 1.00 | 18.16 |
| ATOM | 328 | CA  | CYS | A | 60 | -5.784  | 7.104  | 27.553 | 1.00 | 24.60 |
| ATOM | 329 | CB  | CYS | A | 60 | -5.166  | 7.309  | 28.946 | 1.00 | 22.29 |
| ATOM | 330 | SG  | CYS | A | 60 | -3.478  | 7.963  | 28.894 | 1.00 | 32.87 |
| ATOM | 331 | C   | CYS | A | 60 | -7.200  | 6.568  | 27.701 | 1.00 | 24.69 |
| ATOM | 332 | O   | CYS | A | 60 | -7.633  | 6.163  | 28.783 | 1.00 | 15.41 |
| ATOM | 333 | N   | ASP | A | 61 | -7.989  | 6.554  | 26.627 | 1.00 | 21.29 |
| ATOM | 334 | CA  | ASP | A | 61 | -9.399  | 6.222  | 26.803 | 1.00 | 17.62 |
| ATOM | 335 | CB  | ASP | A | 61 | -10.193 | 6.519  | 25.524 | 1.00 | 24.76 |
| ATOM | 336 | CG  | ASP | A | 61 | -10.158 | 7.992  | 25.163 | 1.00 | 30.04 |
| ATOM | 337 | OD1 | ASP | A | 61 | -9.946  | 8.844  | 26.050 | 1.00 | 27.96 |
| ATOM | 338 | OD2 | ASP | A | 61 | -10.334 | 8.286  | 23.966 | 1.00 | 30.86 |
| ATOM | 339 | C   | ASP | A | 61 | -9.618  | 4.764  | 27.165 | 1.00 | 22.87 |
| ATOM | 340 | O   | ASP | A | 61 | -10.577 | 4.424  | 27.849 | 1.00 | 23.80 |
| ATOM | 341 | N   | ILE | A | 62 | -8.760  | 3.857  | 26.693 | 1.00 | 17.20 |
| ATOM | 342 | CA  | ILE | A | 62 | -9.073  | 2.454  | 27.018 | 1.00 | 17.76 |
| ATOM | 343 | CB  | ILE | A | 62 | -8.198  | 1.491  | 26.203 | 1.00 | 19.59 |
| ATOM | 344 | CG1 | ILE | A | 62 | -8.434  | 1.614  | 24.694 | 1.00 | 30.45 |
| ATOM | 345 | CD1 | ILE | A | 62 | -9.906  | 1.542  | 24.325 | 1.00 | 29.59 |
| ATOM | 346 | CG2 | ILE | A | 62 | -8.389  | 0.061  | 26.685 | 1.00 | 19.52 |
| ATOM | 347 | C   | ILE | A | 62 | -8.891  | 2.209  | 28.509 | 1.00 | 24.81 |
| ATOM | 348 | O   | ILE | A | 62 | -9.671  | 1.523  | 29.170 | 1.00 | 20.96 |
| ATOM | 349 | N   | ALA | A | 63 | -7.831  | 2.828  | 29.030 | 1.00 | 18.90 |
| ATOM | 350 | CA  | ALA | A | 63 | -7.515  | 2.680  | 30.442 | 1.00 | 17.49 |
| ATOM | 351 | CB  | ALA | A | 63 | -6.214  | 3.420  | 30.729 | 1.00 | 14.17 |
| ATOM | 352 | C   | ALA | A | 63 | -8.646  | 3.193  | 31.321 | 1.00 | 22.60 |
| ATOM | 353 | O   | ALA | A | 63 | -8.776  | 2.756  | 32.467 | 1.00 | 21.69 |
| ATOM | 354 | N   | LEU | A | 64 | -9.433  | 4.106  | 30.768 | 1.00 | 22.09 |
| ATOM | 355 | CA  | LEU | A | 64 | -10.531 | 4.780  | 31.447 | 1.00 | 24.05 |
| ATOM | 356 | CB  | LEU | A | 64 | -10.635 | 6.212  | 30.898 | 1.00 | 20.03 |
| ATOM | 357 | CG  | LEU | A | 64 | -9.562  | 7.184  | 31.388 | 1.00 | 17.09 |
| ATOM | 358 | CD1 | LEU | A | 64 | -9.621  | 8.500  | 30.633 | 1.00 | 23.40 |
| ATOM | 359 | CD2 | LEU | A | 64 | -9.722  | 7.431  | 32.885 | 1.00 | 18.46 |
| ATOM | 360 | C   | LEU | A | 64 | -11.867 | 4.072  | 31.310 | 1.00 | 28.67 |
| ATOM | 361 | O   | LEU | A | 64 | -12.878 | 4.468  | 31.898 | 1.00 | 24.74 |
| ATOM | 362 | N   | LEU | A | 65 | -11.959 | 2.988  | 30.544 | 1.00 | 23.30 |
| ATOM | 363 | CA  | LEU | A | 65 | -13.262 | 2.317  | 30.495 | 1.00 | 26.61 |

**FIGURE 109**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 364 | CB  | LEU | A | 65 | -13.254 | 1.209  | 29.436 | 1.00 | 27.54 |
| ATOM | 365 | CG  | LEU | A | 65 | -12.864 | 1.722  | 28.042 | 1.00 | 27.54 |
| ATOM | 366 | CD1 | LEU | A | 65 | -12.668 | 0.573  | 27.069 | 1.00 | 25.94 |
| ATOM | 367 | CD2 | LEU | A | 65 | -13.911 | 2.707  | 27.542 | 1.00 | 31.37 |
| ATOM | 368 | C   | LEU | A | 65 | -13.622 | 1.772  | 31.869 | 1.00 | 24.88 |
| ATOM | 369 | O   | LEU | A | 65 | -12.743 | 1.361  | 32.617 | 1.00 | 27.17 |
| ATOM | 370 | N   | PRO | A | 66 | -14.907 | 1.798  | 32.204 | 1.00 | 28.42 |
| ATOM | 371 | CA  | PRO | A | 66 | -15.378 | 1.350  | 33.511 | 1.00 | 32.94 |
| ATOM | 372 | CB  | PRO | A | 66 | -16.909 | 1.316  | 33.342 | 1.00 | 34.08 |
| ATOM | 373 | CG  | PRO | A | 66 | -17.188 | 2.301  | 32.262 | 1.00 | 39.92 |
| ATOM | 374 | CD  | PRO | A | 66 | -16.002 | 2.281  | 31.339 | 1.00 | 35.79 |
| ATOM | 375 | C   | PRO | A | 66 | -14.879 | -0.038 | 33.884 | 1.00 | 25.20 |
| ATOM | 376 | O   | PRO | A | 66 | -14.577 | -0.329 | 35.039 | 1.00 | 30.25 |
| ATOM | 377 | N   | GLU | A | 67 | -14.784 | -0.948 | 32.916 | 1.00 | 26.85 |
| ATOM | 378 | CA  | GLU | A | 67 | -14.418 | -2.299 | 33.346 | 1.00 | 35.73 |
| ATOM | 379 | CB  | GLU | A | 67 | -14.879 | -3.321 | 32.308 | 1.00 | 39.08 |
| ATOM | 380 | CG  | GLU | A | 67 | -15.067 | -2.754 | 30.914 | 1.00 | 48.88 |
| ATOM | 381 | CD  | GLU | A | 67 | -14.264 | -3.501 | 29.864 | 1.00 | 57.56 |
| ATOM | 382 | OE1 | GLU | A | 67 | -14.251 | -4.752 | 29.884 | 1.00 | 77.10 |
| ATOM | 383 | OE2 | GLU | A | 67 | -13.642 | -2.832 | 29.012 | 1.00 | 41.80 |
| ATOM | 384 | C   | GLU | A | 67 | -12.923 | -2.398 | 33.622 | 1.00 | 36.25 |
| ATOM | 385 | O   | GLU | A | 67 | -12.447 | -3.441 | 34.078 | 1.00 | 32.32 |
| ATOM | 386 | N   | ASN | A | 68 | -12.167 | -1.333 | 33.359 | 1.00 | 31.47 |
| ATOM | 387 | CA  | ASN | A | 68 | -10.724 | -1.380 | 33.588 | 1.00 | 21.87 |
| ATOM | 388 | CB  | ASN | A | 68 | -9.950  | -0.794 | 32.395 | 1.00 | 22.35 |
| ATOM | 389 | CG  | ASN | A | 68 | -10.008 | -1.714 | 31.195 | 1.00 | 19.79 |
| ATOM | 390 | OD1 | ASN | A | 68 | -10.127 | -2.930 | 31.350 | 1.00 | 23.52 |
| ATOM | 391 | ND2 | ASN | A | 68 | -9.927  | -1.147 | 29.997 | 1.00 | 19.33 |
| ATOM | 392 | C   | ASN | A | 68 | -10.329 | -0.618 | 34.841 | 1.00 | 20.30 |
| ATOM | 393 | O   | ASN | A | 68 | -9.154  | -0.604 | 35.215 | 1.00 | 22.70 |
| ATOM | 394 | N   | ARG | A | 69 | -11.286 | 0.026  | 35.508 | 1.00 | 26.70 |
| ATOM | 395 | CA  | ARG | A | 69 | -10.894 | 0.889  | 36.623 | 1.00 | 33.64 |
| ATOM | 396 | CB  | ARG | A | 69 | -12.116 | 1.607  | 37.211 | 1.00 | 44.80 |
| ATOM | 397 | CG  | ARG | A | 69 | -11.775 | 2.959  | 37.824 | 1.00 | 54.18 |
| ATOM | 398 | CD  | ARG | A | 69 | -12.982 | 3.581  | 38.508 | 1.00 | 63.01 |
| ATOM | 399 | NE  | ARG | A | 69 | -12.717 | 3.903  | 39.904 | 1.00 | 71.32 |
| ATOM | 400 | CZ  | ARG | A | 69 | -13.573 | 3.781  | 40.910 | 1.00 | 77.50 |
| ATOM | 401 | NH1 | ARG | A | 69 | -14.801 | 3.330  | 40.694 | 1.00 | 86.91 |
| ATOM | 402 | NH2 | ARG | A | 69 | -13.203 | 4.108  | 42.144 | 1.00 | 73.55 |
| ATOM | 403 | C   | ARG | A | 69 | -10.153 | 0.129  | 37.715 | 1.00 | 29.65 |
| ATOM | 404 | O   | ARG | A | 69 | -9.113  | 0.604  | 38.189 | 1.00 | 40.10 |
| ATOM | 405 | N   | GLY | A | 70 | -10.644 | -1.040 | 38.113 | 1.00 | 23.99 |
| ATOM | 406 | CA  | GLY | A | 70 | -9.961  | -1.818 | 39.143 | 1.00 | 19.86 |
| ATOM | 407 | C   | GLY | A | 70 | -8.590  | -2.288 | 38.689 | 1.00 | 24.39 |
| ATOM | 408 | O   | GLY | A | 70 | -7.784  | -2.734 | 39.521 | 1.00 | 22.56 |
| ATOM | 409 | N   | LYS | A | 71 | -8.301  | -2.205 | 37.379 | 1.00 | 19.98 |
| ATOM | 410 | CA  | LYS | A | 71 | -7.003  | -2.702 | 36.908 | 1.00 | 15.60 |
| ATOM | 411 | CB  | LYS | A | 71 | -7.123  | -3.252 | 35.480 | 1.00 | 18.68 |
| ATOM | 412 | CG  | LYS | A | 71 | -8.200  | -4.318 | 35.326 | 1.00 | 15.28 |
| ATOM | 413 | CD  | LYS | A | 71 | -8.403  | -4.675 | 33.855 | 1.00 | 15.32 |
| ATOM | 414 | CE  | LYS | A | 71 | -9.713  | -5.448 | 33.703 | 1.00 | 27.04 |
| ATOM | 415 | NZ  | LYS | A | 71 | -10.141 | -5.554 | 32.281 | 1.00 | 31.96 |

**FIGURE 110**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 416 | C   | LYS | A | 71 | -5.890 | -1.672 | 36.944 | 1.00 | 14.54 |
| ATOM | 417 | O   | LYS | A | 71 | -4.752 | -1.993 | 36.578 | 1.00 | 17.52 |
| ATOM | 418 | N   | ASN | A | 72 | -6.149 | -0.439 | 37.371 | 1.00 | 11.96 |
| ATOM | 419 | CA  | ASN | A | 72 | -5.101 | 0.568  | 37.479 | 1.00 | 11.74 |
| ATOM | 420 | CB  | ASN | A | 72 | -5.545 | 1.876  | 36.813 | 1.00 | 14.82 |
| ATOM | 421 | CG  | ASN | A | 72 | -5.837 | 1.654  | 35.339 | 1.00 | 23.46 |
| ATOM | 422 | OD1 | ASN | A | 72 | -5.007 | 1.128  | 34.599 | 1.00 | 16.09 |
| ATOM | 423 | ND2 | ASN | A | 72 | -7.025 | 2.057  | 34.903 | 1.00 | 21.08 |
| ATOM | 424 | C   | ASN | A | 72 | -4.753 | 0.835  | 38.937 | 1.00 | 16.08 |
| ATOM | 425 | O   | ASN | A | 72 | -5.647 | 1.079  | 39.741 | 1.00 | 18.28 |
| ATOM | 426 | N   | ARG | A | 73 | -3.471 | 0.788  | 39.258 | 1.00 | 12.51 |
| ATOM | 427 | CA  | ARG | A | 73 | -3.013 | 1.010  | 40.621 | 1.00 | 20.92 |
| ATOM | 428 | CB  | ARG | A | 73 | -1.525 | 0.666  | 40.738 | 1.00 | 13.10 |
| ATOM | 429 | CG  | ARG | A | 73 | -0.989 | 0.829  | 42.148 | 1.00 | 9.31  |
| ATOM | 430 | CD  | ARG | A | 73 | 0.454  | 0.359  | 42.272 | 1.00 | 11.98 |
| ATOM | 431 | NE  | ARG | A | 73 | 0.510  | -1.117 | 42.294 | 1.00 | 9.41  |
| ATOM | 432 | CZ  | ARG | A | 73 | 0.265  | -1.768 | 43.428 | 1.00 | 17.50 |
| ATOM | 433 | NH1 | ARG | A | 73 | -0.024 | -1.096 | 44.549 | 1.00 | 14.11 |
| ATOM | 434 | NH2 | ARG | A | 73 | 0.330  | -3.094 | 43.391 | 1.00 | 16.87 |
| ATOM | 435 | C   | ARG | A | 73 | -3.255 | 2.460  | 41.041 | 1.00 | 25.16 |
| ATOM | 436 | O   | ARG | A | 73 | -3.658 | 2.737  | 42.170 | 1.00 | 14.89 |
| ATOM | 437 | N   | TYR | A | 74 | -2.991 | 3.373  | 40.114 | 1.00 | 17.87 |
| ATOM | 438 | CA  | TYR | A | 74 | -3.209 | 4.806  | 40.336 | 1.00 | 15.26 |
| ATOM | 439 | CB  | TYR | A | 74 | -1.887 | 5.539  | 40.348 | 1.00 | 18.93 |
| ATOM | 440 | CG  | TYR | A | 74 | -0.898 | 5.054  | 41.388 | 1.00 | 19.16 |
| ATOM | 441 | CD1 | TYR | A | 74 | -1.081 | 5.313  | 42.735 | 1.00 | 22.07 |
| ATOM | 442 | CE1 | TYR | A | 74 | -0.174 | 4.871  | 43.684 | 1.00 | 17.71 |
| ATOM | 443 | CZ  | TYR | A | 74 | 0.932  | 4.160  | 43.289 | 1.00 | 16.94 |
| ATOM | 444 | OH  | TYR | A | 74 | 1.851  | 3.713  | 44.213 | 1.00 | 16.65 |
| ATOM | 445 | CE2 | TYR | A | 74 | 1.139  | 3.891  | 41.947 | 1.00 | 20.51 |
| ATOM | 446 | CD2 | TYR | A | 74 | 0.225  | 4.337  | 41.009 | 1.00 | 14.89 |
| ATOM | 447 | C   | TYR | A | 74 | -4.150 | 5.322  | 39.263 | 1.00 | 23.96 |
| ATOM | 448 | O   | TYR | A | 74 | -3.994 | 5.065  | 38.065 | 1.00 | 19.22 |
| ATOM | 449 | N   | ASN | A | 75 | -5.202 | 6.053  | 39.641 | 1.00 | 18.99 |
| ATOM | 450 | CA  | ASN | A | 75 | -6.220 | 6.288  | 38.610 | 1.00 | 23.42 |
| ATOM | 451 | CB  | ASN | A | 75 | -7.557 | 6.585  | 39.296 | 1.00 | 34.45 |
| ATOM | 452 | CG  | ASN | A | 75 | -8.137 | 5.350  | 39.975 | 1.00 | 51.03 |
| ATOM | 453 | OD1 | ASN | A | 75 | -8.673 | 5.414  | 41.085 | 1.00 | 50.00 |
| ATOM | 454 | ND2 | ASN | A | 75 | -8.051 | 4.180  | 39.342 | 1.00 | 38.85 |
| ATOM | 455 | C   | ASN | A | 75 | -5.736 | 7.353  | 37.640 | 1.00 | 18.82 |
| ATOM | 456 | O   | ASN | A | 75 | -6.317 | 7.585  | 36.580 | 1.00 | 20.63 |
| ATOM | 457 | N   | ASN | A | 76 | -4.615 | 7.991  | 37.977 | 1.00 | 16.28 |
| ATOM | 458 | CA  | ASN | A | 76 | -4.105 | 9.045  | 37.110 | 1.00 | 19.45 |
| ATOM | 459 | CB  | ASN | A | 76 | -3.997 | 10.339 | 37.926 | 1.00 | 22.45 |
| ATOM | 460 | CG  | ASN | A | 76 | -2.980 | 10.295 | 39.044 | 1.00 | 33.59 |
| ATOM | 461 | OD1 | ASN | A | 76 | -2.679 | 9.257  | 39.636 | 1.00 | 26.17 |
| ATOM | 462 | ND2 | ASN | A | 76 | -2.431 | 11.474 | 39.344 | 1.00 | 29.60 |
| ATOM | 463 | C   | ASN | A | 76 | -2.781 | 8.692  | 36.465 | 1.00 | 17.17 |
| ATOM | 464 | O   | ASN | A | 76 | -2.066 | 9.532  | 35.917 | 1.00 | 17.91 |
| ATOM | 465 | N   | ILE | A | 77 | -2.389 | 7.423  | 36.475 | 1.00 | 20.00 |
| ATOM | 466 | CA  | ILE | A | 77 | -1.171 | 6.992  | 35.791 | 1.00 | 14.81 |
| ATOM | 467 | CB  | ILE | A | 77 | -0.049 | 6.504  | 36.702 | 1.00 | 11.59 |

**FIGURE 111**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 468 | CG1 | ILE | A | 77 | 0.336  | 7.468  | 37.832 | 1.00 | 17.04 |
| ATOM | 469 | CD1 | ILE | A | 77 | 0.986  | 8.713  | 37.282 | 1.00 | 17.56 |
| ATOM | 470 | CG2 | ILE | A | 77 | 1.227  | 6.165  | 35.924 | 1.00 | 15.42 |
| ATOM | 471 | C   | ILE | A | 77 | -1.617 | 5.835  | 34.878 | 1.00 | 16.96 |
| ATOM | 472 | O   | ILE | A | 77 | -1.733 | 4.718  | 35.381 | 1.00 | 15.55 |
| ATOM | 473 | N   | LEU | A | 78 | -1.897 | 6.184  | 33.632 | 1.00 | 12.76 |
| ATOM | 474 | CA  | LEU | A | 78 | -2.530 | 5.255  | 32.689 | 1.00 | 10.94 |
| ATOM | 475 | CB  | LEU | A | 78 | -3.984 | 5.623  | 32.413 | 1.00 | 12.51 |
| ATOM | 476 | CG  | LEU | A | 78 | -4.880 | 5.963  | 33.601 | 1.00 | 19.43 |
| ATOM | 477 | CD1 | LEU | A | 78 | -6.237 | 6.497  | 33.151 | 1.00 | 22.19 |
| ATOM | 478 | CD2 | LEU | A | 78 | -5.082 | 4.744  | 34.486 | 1.00 | 24.35 |
| ATOM | 479 | C   | LEU | A | 78 | -1.723 | 5.244  | 31.398 | 1.00 | 17.94 |
| ATOM | 480 | O   | LEU | A | 78 | -1.093 | 6.248  | 31.056 | 1.00 | 16.73 |
| ATOM | 481 | N   | PRO | A | 79 | -1.711 | 4.123  | 30.692 | 1.00 | 19.09 |
| ATOM | 482 | CA  | PRO | A | 79 | -0.920 | 4.050  | 29.450 | 1.00 | 16.12 |
| ATOM | 483 | CB  | PRO | A | 79 | -0.870 | 2.539  | 29.199 | 1.00 | 9.23  |
| ATOM | 484 | CG  | PRO | A | 79 | -2.204 | 2.074  | 29.718 | 1.00 | 11.75 |
| ATOM | 485 | CD  | PRO | A | 79 | -2.411 | 2.860  | 30.988 | 1.00 | 15.77 |
| ATOM | 486 | C   | PRO | A | 79 | -1.655 | 4.794  | 28.339 | 1.00 | 15.99 |
| ATOM | 487 | O   | PRO | A | 79 | -2.893 | 4.828  | 28.388 | 1.00 | 15.25 |
| ATOM | 488 | N   | TYR | A | 80 | -0.926 | 5.362  | 27.389 | 1.00 | 10.13 |
| ATOM | 489 | CA  | TYR | A | 80 | -1.502 | 5.993  | 26.206 | 1.00 | 11.18 |
| ATOM | 490 | CB  | TYR | A | 80 | -0.451 | 6.764  | 25.423 | 1.00 | 13.27 |
| ATOM | 491 | CG  | TYR | A | 80 | 0.146  | 7.959  | 26.117 | 1.00 | 12.63 |
| ATOM | 492 | CD1 | TYR | A | 80 | -0.697 | 8.902  | 26.685 | 1.00 | 18.08 |
| ATOM | 493 | CE1 | TYR | A | 80 | -0.173 | 10.005 | 27.321 | 1.00 | 20.03 |
| ATOM | 494 | CZ  | TYR | A | 80 | 1.186  | 10.172 | 27.391 | 1.00 | 16.07 |
| ATOM | 495 | OH  | TYR | A | 80 | 1.682  | 11.281 | 28.032 | 1.00 | 21.65 |
| ATOM | 496 | CE2 | TYR | A | 80 | 2.054  | 9.257  | 26.837 | 1.00 | 13.46 |
| ATOM | 497 | CD2 | TYR | A | 80 | 1.507  | 8.150  | 26.198 | 1.00 | 14.05 |
| ATOM | 498 | C   | TYR | A | 80 | -2.104 | 4.930  | 25.286 | 1.00 | 18.00 |
| ATOM | 499 | O   | TYR | A | 80 | -1.568 | 3.823  | 25.165 | 1.00 | 15.44 |
| ATOM | 500 | N   | ASP | A | 81 | -3.222 | 5.206  | 24.625 | 1.00 | 15.66 |
| ATOM | 501 | CA  | ASP | A | 81 | -3.849 | 4.129  | 23.846 | 1.00 | 18.95 |
| ATOM | 502 | CB  | ASP | A | 81 | -5.184 | 4.541  | 23.239 | 1.00 | 21.06 |
| ATOM | 503 | CG  | ASP | A | 81 | -6.217 | 5.004  | 24.239 | 1.00 | 23.24 |
| ATOM | 504 | OD1 | ASP | A | 81 | -6.322 | 4.394  | 25.318 | 1.00 | 20.28 |
| ATOM | 505 | OD2 | ASP | A | 81 | -6.944 | 5.971  | 23.937 | 1.00 | 21.10 |
| ATOM | 506 | C   | ASP | A | 81 | -2.919 | 3.699  | 22.717 | 1.00 | 19.22 |
| ATOM | 507 | O   | ASP | A | 81 | -2.884 | 2.543  | 22.314 | 1.00 | 24.23 |
| ATOM | 508 | N   | ALA | A | 82 | -2.171 | 4.664  | 22.193 | 1.00 | 20.83 |
| ATOM | 509 | CA  | ALA | A | 82 | -1.326 | 4.375  | 21.033 | 1.00 | 21.56 |
| ATOM | 510 | CB  | ALA | A | 82 | -0.802 | 5.697  | 20.471 | 1.00 | 18.25 |
| ATOM | 511 | C   | ALA | A | 82 | -0.179 | 3.424  | 21.333 | 1.00 | 17.70 |
| ATOM | 512 | O   | ALA | A | 82 | 0.344  | 2.784  | 20.412 | 1.00 | 24.59 |
| ATOM | 513 | N   | THR | A | 83 | 0.291  | 3.282  | 22.570 | 1.00 | 14.11 |
| ATOM | 514 | CA  | THR | A | 83 | 1.482  | 2.482  | 22.831 | 1.00 | 15.16 |
| ATOM | 515 | CB  | THR | A | 83 | 2.667  | 3.349  | 23.283 | 1.00 | 26.72 |
| ATOM | 516 | OG1 | THR | A | 83 | 2.291  | 4.126  | 24.431 | 1.00 | 20.70 |
| ATOM | 517 | CG2 | THR | A | 83 | 3.076  | 4.358  | 22.213 | 1.00 | 24.85 |
| ATOM | 518 | C   | THR | A | 83 | 1.223  | 1.437  | 23.918 | 1.00 | 17.17 |
| ATOM | 519 | O   | THR | A | 83 | 2.168  | 0.825  | 24.412 | 1.00 | 17.29 |

**FIGURE 112**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |         |        |      |        |
|------|-----|-----|-----|---|----|---------|---------|--------|------|--------|
| ATOM | 520 | N   | ARG | A | 84 | -0.030  | 1.226   | 24.310 | 1.00 | 14.78  |
| ATOM | 521 | CA  | ARG | A | 84 | -0.304  | 0.265   | 25.377 | 1.00 | 14.16  |
| ATOM | 522 | CB  | ARG | A | 84 | -1.752  | 0.389   | 25.832 | 1.00 | 16.16  |
| ATOM | 523 | CG  | ARG | A | 84 | -2.824  | -0.021  | 24.841 | 1.00 | 12.30  |
| ATOM | 524 | CD  | ARG | A | 84 | -4.206  | 0.035   | 25.483 | 1.00 | 18.81  |
| ATOM | 525 | NE  | ARG | A | 84 | -5.231  | -0.504  | 24.587 | 1.00 | 18.67  |
| ATOM | 526 | CZ  | ARG | A | 84 | -5.856  | -1.657  | 24.745 | 1.00 | 25.65  |
| ATOM | 527 | NH1 | ARG | A | 84 | -5.570  | -2.421  | 25.794 | 1.00 | 18.24  |
| ATOM | 528 | NH2 | ARG | A | 84 | -6.769  | -2.038  | 23.856 | 1.00 | 23.18  |
| ATOM | 529 | C   | ARG | A | 84 | 0.002   | -1.164  | 24.926 | 1.00 | 19.54  |
| ATOM | 530 | O   | ARG | A | 84 | -0.053  | -1.498  | 23.748 | 1.00 | 16.47  |
| ATOM | 531 | N   | VAL | A | 85 | 0.340   | -2.027  | 25.871 | 1.00 | 14.56  |
| ATOM | 532 | CA  | VAL | A | 85 | 0.511   | -3.453  | 25.593 | 1.00 | 15.91  |
| ATOM | 533 | CB  | VAL | A | 85 | 1.516   | -4.099  | 26.552 | 1.00 | 9.66   |
| ATOM | 534 | CG1 | VAL | A | 85 | 1.595   | -5.605  | 26.279 | 1.00 | 26.22  |
| ATOM | 535 | CG2 | VAL | A | 85 | 2.900   | -3.489  | 26.419 | 1.00 | 8.35   |
| ATOM | 536 | C   | VAL | A | 85 | -0.824  | -4.164  | 25.708 | 1.00 | 18.09  |
| ATOM | 537 | O   | VAL | A | 85 | -1.596  | -4.001  | 26.664 | 1.00 | 17.84  |
| ATOM | 538 | N   | LYS | A | 86 | -1.170  | -4.991  | 24.713 | 1.00 | 17.85  |
| ATOM | 539 | CA  | LYS | A | 86 | -2.481  | -5.634  | 24.797 | 1.00 | 16.55  |
| ATOM | 540 | CB  | LYS | A | 86 | -3.270  | -5.448  | 23.499 | 1.00 | 22.98  |
| ATOM | 541 | CG  | LYS | A | 86 | -3.353  | -4.027  | 22.972 | 1.00 | 25.37  |
| ATOM | 542 | CD  | LYS | A | 86 | -4.093  | -3.996  | 21.641 | 1.00 | 35.98  |
| ATOM | 543 | CE  | LYS | A | 86 | -4.302  | -2.569  | 21.152 | 1.00 | 41.61  |
| ATOM | 544 | NZ  | LYS | A | 86 | -5.067  | -2.535  | 19.870 | 1.00 | 41.47  |
| ATOM | 545 | C   | LYS | A | 86 | -2.354  | -7.130  | 25.073 | 1.00 | 17.71  |
| ATOM | 546 | O   | LYS | A | 86 | -1.473  | -7.780  | 24.495 | 1.00 | 26.73  |
| ATOM | 547 | N   | LEU | A | 87 | -3.238  | -7.641  | 25.909 | 1.00 | 16.65  |
| ATOM | 548 | CA  | LEU | A | 87 | -3.386  | -9.070  | 26.157 | 1.00 | 21.87  |
| ATOM | 549 | CB  | LEU | A | 87 | -4.108  | -9.340  | 27.477 | 1.00 | 22.56  |
| ATOM | 550 | CG  | LEU | A | 87 | -3.573  | -8.679  | 28.751 | 1.00 | 19.45  |
| ATOM | 551 | CD1 | LEU | A | 87 | -4.502  | -8.981  | 29.920 | 1.00 | 33.41  |
| ATOM | 552 | CD2 | LEU | A | 87 | -2.155  | -9.123  | 29.057 | 1.00 | 19.25  |
| ATOM | 553 | C   | LEU | A | 87 | -4.194  | -9.716  | 25.033 | 1.00 | 34.42  |
| ATOM | 554 | O   | LEU | A | 87 | -5.103  | -9.087  | 24.480 | 1.00 | 29.92  |
| ATOM | 555 | N   | SER | A | 88 | -3.906  | -10.961 | 24.684 | 1.00 | 39.81  |
| ATOM | 556 | CA  | SER | A | 88 | -4.712  | -11.686 | 23.715 | 1.00 | 42.02  |
| ATOM | 557 | CB  | SER | A | 88 | -4.153  | -13.103 | 23.509 | 1.00 | 45.96  |
| ATOM | 558 | OG  | SER | A | 88 | -4.499  | -13.843 | 24.684 | 1.00 | 44.96  |
| ATOM | 559 | C   | SER | A | 88 | -6.154  | -11.853 | 24.182 | 1.00 | 39.54  |
| ATOM | 560 | O   | SER | A | 88 | -6.425  | -11.712 | 25.374 | 1.00 | 35.93  |
| ATOM | 561 | N   | ASN | A | 89 | -7.041  | -12.175 | 23.251 | 1.00 | 58.52  |
| ATOM | 562 | CA  | ASN | A | 89 | -8.435  | -12.501 | 23.518 | 1.00 | 76.46  |
| ATOM | 563 | CB  | ASN | A | 89 | -9.366  | -11.396 | 23.017 | 1.00 | 82.65  |
| ATOM | 564 | CG  | ASN | A | 89 | -9.457  | -11.372 | 21.501 | 1.00 | 93.50  |
| ATOM | 565 | OD1 | ASN | A | 89 | -10.512 | -11.100 | 20.929 | 1.00 | 104.34 |
| ATOM | 566 | ND2 | ASN | A | 89 | -8.337  | -11.659 | 20.847 | 1.00 | 109.77 |
| ATOM | 567 | C   | ASN | A | 89 | -8.807  | -13.831 | 22.860 | 1.00 | 88.77  |
| ATOM | 568 | O   | ASN | A | 89 | -8.533  | -14.011 | 21.671 | 1.00 | 92.19  |
| ATOM | 569 | N   | VAL | A | 90 | -9.407  | -14.736 | 23.621 | 1.00 | 99.23  |
| ATOM | 570 | CA  | VAL | A | 90 | -9.793  | -16.059 | 23.144 | 1.00 | 106.42 |
| ATOM | 571 | CB  | VAL | A | 90 | -8.923  | -17.172 | 23.760 | 1.00 | 106.95 |

**FIGURE 113**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |         |        |            |
|------|-----|-----|-----|---|----|---------|---------|--------|------------|
| ATOM | 572 | CG1 | VAL | A | 90 | -9.298  | -18.525 | 23.172 | 1.00112.12 |
| ATOM | 573 | CG2 | VAL | A | 90 | -7.444  | -16.892 | 23.548 | 1.00105.34 |
| ATOM | 574 | C   | VAL | A | 90 | -11.258 | -16.369 | 23.451 | 1.00111.33 |
| ATOM | 575 | O   | VAL | A | 90 | -12.138 | -16.117 | 22.628 | 1.00105.84 |
| ATOM | 576 | N   | ASP | A | 91 | -11.510 | -16.921 | 24.632 | 1.00119.26 |
| ATOM | 577 | CA  | ASP | A | 91 | -12.855 | -17.239 | 25.095 | 1.00128.16 |
| ATOM | 578 | CB  | ASP | A | 91 | -12.828 | -18.448 | 26.031 | 1.00125.07 |
| ATOM | 579 | CG  | ASP | A | 91 | -14.191 | -18.774 | 26.609 | 1.00121.16 |
| ATOM | 580 | OD1 | ASP | A | 91 | -15.007 | -19.377 | 25.880 | 1.00104.75 |
| ATOM | 581 | OD2 | ASP | A | 91 | -14.447 | -18.433 | 27.785 | 1.00117.18 |
| ATOM | 582 | C   | ASP | A | 91 | -13.482 | -16.042 | 25.807 | 1.00139.13 |
| ATOM | 583 | O   | ASP | A | 91 | -13.028 | -15.676 | 26.894 | 1.00148.32 |
| ATOM | 584 | N   | ASP | A | 92 | -14.503 | -15.447 | 25.202 | 1.00145.93 |
| ATOM | 585 | CA  | ASP | A | 92 | -15.147 | -14.241 | 25.726 | 1.00149.70 |
| ATOM | 586 | CB  | ASP | A | 92 | -15.415 | -14.375 | 27.225 | 1.00149.57 |
| ATOM | 587 | CG  | ASP | A | 92 | -16.361 | -15.502 | 27.584 | 1.00147.36 |
| ATOM | 588 | OD1 | ASP | A | 92 | -17.567 | -15.233 | 27.781 | 1.00137.75 |
| ATOM | 589 | OD2 | ASP | A | 92 | -15.912 | -16.665 | 27.677 | 1.00148.40 |
| ATOM | 590 | C   | ASP | A | 92 | -14.286 | -13.021 | 25.419 | 1.00150.50 |
| ATOM | 591 | O   | ASP | A | 92 | -13.148 | -12.934 | 25.892 | 1.00155.89 |
| ATOM | 592 | N   | ASP | A | 93 | -14.778 | -12.068 | 24.620 | 1.00148.19 |
| ATOM | 593 | CA  | ASP | A | 93 | -13.886 | -10.998 | 24.173 | 1.00145.42 |
| ATOM | 594 | CB  | ASP | A | 93 | -13.545 | -11.222 | 22.687 | 1.00146.89 |
| ATOM | 595 | CG  | ASP | A | 93 | -14.744 | -11.594 | 21.844 | 1.00147.24 |
| ATOM | 596 | OD1 | ASP | A | 93 | -15.278 | -12.710 | 22.011 | 1.00141.98 |
| ATOM | 597 | OD2 | ASP | A | 93 | -15.159 | -10.772 | 21.001 | 1.00148.93 |
| ATOM | 598 | C   | ASP | A | 93 | -14.404 | -9.578  | 24.346 | 1.00140.50 |
| ATOM | 599 | O   | ASP | A | 93 | -14.742 | -8.922  | 23.357 | 1.00135.04 |
| ATOM | 600 | N   | PRO | A | 94 | -14.451 | -9.070  | 25.570 | 1.00137.75 |
| ATOM | 601 | CA  | PRO | A | 94 | -14.684 | -7.638  | 25.812 | 1.00134.16 |
| ATOM | 602 | CB  | PRO | A | 94 | -15.340 | -7.646  | 27.190 | 1.00136.91 |
| ATOM | 603 | CG  | PRO | A | 94 | -14.801 | -8.848  | 27.882 | 1.00138.06 |
| ATOM | 604 | CD  | PRO | A | 94 | -14.305 | -9.803  | 26.837 | 1.00139.01 |
| ATOM | 605 | C   | PRO | A | 94 | -13.363 | -6.879  | 25.830 | 1.00126.58 |
| ATOM | 606 | O   | PRO | A | 94 | -12.437 | -7.253  | 25.099 | 1.00132.66 |
| ATOM | 607 | N   | CYS | A | 95 | -13.220 | -5.827  | 26.639 | 1.00114.33 |
| ATOM | 608 | CA  | CYS | A | 95 | -11.898 | -5.198  | 26.765 | 1.00 95.06 |
| ATOM | 609 | CB  | CYS | A | 95 | -11.947 | -3.690  | 26.961 | 1.00 97.01 |
| ATOM | 610 | SG  | CYS | A | 95 | -10.323 | -2.901  | 27.121 | 1.00 74.50 |
| ATOM | 611 | C   | CYS | A | 95 | -11.146 | -5.872  | 27.913 | 1.00 71.83 |
| ATOM | 612 | O   | CYS | A | 95 | -10.629 | -5.311  | 28.870 | 1.00 58.75 |
| ATOM | 613 | N   | SER | A | 96 | -11.089 | -7.193  | 27.759 | 1.00 54.83 |
| ATOM | 614 | CA  | SER | A | 96 | -10.254 | -8.038  | 28.595 | 1.00 46.09 |
| ATOM | 615 | CB  | SER | A | 96 | -10.848 | -9.437  | 28.720 | 1.00 49.86 |
| ATOM | 616 | OG  | SER | A | 96 | -10.801 | -10.147 | 27.491 | 1.00 47.97 |
| ATOM | 617 | C   | SER | A | 96 | -8.854  | -8.076  | 27.988 | 1.00 31.56 |
| ATOM | 618 | O   | SER | A | 96 | -8.045  | -8.933  | 28.321 | 1.00 30.50 |
| ATOM | 619 | N   | ASP | A | 97 | -8.562  | -7.129  | 27.085 | 1.00 25.83 |
| ATOM | 620 | CA  | ASP | A | 97 | -7.233  | -7.050  | 26.495 | 1.00 17.26 |
| ATOM | 621 | CB  | ASP | A | 97 | -7.317  | -6.646  | 25.029 | 1.00 22.22 |
| ATOM | 622 | CG  | ASP | A | 97 | -7.590  | -5.179  | 24.772 | 1.00 32.54 |
| ATOM | 623 | OD1 | ASP | A | 97 | -7.945  | -4.404  | 25.681 | 1.00 25.44 |

**FIGURE 114**

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 624 | OD2 | ASP | A | 97  | -7.444 | -4.765 | 23.600 | 1.00 | 44.31 |
| ATOM | 625 | C   | ASP | A | 97  | -6.357 | -6.065 | 27.271 | 1.00 | 18.88 |
| ATOM | 626 | O   | ASP | A | 97  | -5.194 | -5.883 | 26.902 | 1.00 | 18.89 |
| ATOM | 627 | N   | TYR | A | 98  | -6.947 | -5.456 | 28.296 | 1.00 | 20.04 |
| ATOM | 628 | CA  | TYR | A | 98  | -6.313 | -4.338 | 28.976 | 1.00 | 18.41 |
| ATOM | 629 | CB  | TYR | A | 98  | -7.366 | -3.378 | 29.609 | 1.00 | 18.59 |
| ATOM | 630 | CG  | TYR | A | 98  | -6.631 | -2.221 | 30.288 | 1.00 | 20.03 |
| ATOM | 631 | CD1 | TYR | A | 98  | -6.043 | -1.216 | 29.522 | 1.00 | 16.83 |
| ATOM | 632 | CE1 | TYR | A | 98  | -5.361 | -0.144 | 30.090 | 1.00 | 13.49 |
| ATOM | 633 | CZ  | TYR | A | 98  | -5.276 | -0.116 | 31.471 | 1.00 | 19.51 |
| ATOM | 634 | OH  | TYR | A | 98  | -4.624 | 0.908  | 32.106 | 1.00 | 14.09 |
| ATOM | 635 | CE2 | TYR | A | 98  | -5.846 | -1.095 | 32.255 | 1.00 | 13.64 |
| ATOM | 636 | CD2 | TYR | A | 98  | -6.528 | -2.145 | 31.673 | 1.00 | 17.45 |
| ATOM | 637 | C   | TYR | A | 98  | -5.343 | -4.746 | 30.066 | 1.00 | 18.17 |
| ATOM | 638 | O   | TYR | A | 98  | -5.664 | -5.449 | 31.020 | 1.00 | 22.86 |
| ATOM | 639 | N   | ILE | A | 99  | -4.130 | -4.218 | 29.989 | 1.00 | 14.66 |
| ATOM | 640 | CA  | ILE | A | 99  | -3.274 | -4.175 | 31.172 | 1.00 | 17.87 |
| ATOM | 641 | CB  | ILE | A | 99  | -2.221 | -5.290 | 31.223 | 1.00 | 17.34 |
| ATOM | 642 | CG1 | ILE | A | 99  | -1.274 | -5.190 | 32.428 | 1.00 | 13.76 |
| ATOM | 643 | CD1 | ILE | A | 99  | -0.492 | -6.481 | 32.633 | 1.00 | 14.80 |
| ATOM | 644 | CG2 | ILE | A | 99  | -1.443 | -5.348 | 29.924 | 1.00 | 15.59 |
| ATOM | 645 | C   | ILE | A | 99  | -2.594 | -2.807 | 31.227 | 1.00 | 14.26 |
| ATOM | 646 | O   | ILE | A | 99  | -2.353 | -2.191 | 30.183 | 1.00 | 16.44 |
| ATOM | 647 | N   | ASN | A | 100 | -2.315 | -2.334 | 32.435 | 1.00 | 14.80 |
| ATOM | 648 | CA  | ASN | A | 100 | -1.609 | -1.054 | 32.562 | 1.00 | 12.64 |
| ATOM | 649 | CB  | ASN | A | 100 | -1.818 | -0.440 | 33.951 | 1.00 | 11.26 |
| ATOM | 650 | CG  | ASN | A | 100 | -1.326 | 0.997  | 33.976 | 1.00 | 13.09 |
| ATOM | 651 | OD1 | ASN | A | 100 | -0.260 | 1.278  | 33.456 | 1.00 | 13.19 |
| ATOM | 652 | ND2 | ASN | A | 100 | -2.099 | 1.903  | 34.579 | 1.00 | 15.88 |
| ATOM | 653 | C   | ASN | A | 100 | -0.134 | -1.242 | 32.244 | 1.00 | 10.03 |
| ATOM | 654 | O   | ASN | A | 100 | 0.698  | -1.477 | 33.119 | 1.00 | 12.85 |
| ATOM | 655 | N   | ALA | A | 101 | 0.193  | -1.152 | 30.946 | 1.00 | 10.66 |
| ATOM | 656 | CA  | ALA | A | 101 | 1.550  | -1.361 | 30.488 | 1.00 | 9.30  |
| ATOM | 657 | CB  | ALA | A | 101 | 1.839  | -2.863 | 30.397 | 1.00 | 13.80 |
| ATOM | 658 | C   | ALA | A | 101 | 1.777  | -0.712 | 29.125 | 1.00 | 6.85  |
| ATOM | 659 | O   | ALA | A | 101 | 0.809  | -0.539 | 28.394 | 1.00 | 12.08 |
| ATOM | 660 | N   | SER | A | 102 | 3.026  | -0.393 | 28.829 | 1.00 | 9.92  |
| ATOM | 661 | CA  | SER | A | 102 | 3.389  | 0.362  | 27.641 | 1.00 | 14.73 |
| ATOM | 662 | CB  | SER | A | 102 | 3.650  | 1.831  | 28.010 | 1.00 | 11.60 |
| ATOM | 663 | OG  | SER | A | 102 | 2.561  | 2.407  | 28.691 | 1.00 | 11.12 |
| ATOM | 664 | C   | SER | A | 102 | 4.644  | -0.211 | 26.986 | 1.00 | 15.69 |
| ATOM | 665 | O   | SER | A | 102 | 5.563  | -0.654 | 27.686 | 1.00 | 12.17 |
| ATOM | 666 | N   | TYR | A | 103 | 4.680  | -0.176 | 25.652 | 1.00 | 9.06  |
| ATOM | 667 | CA  | TYR | A | 103 | 5.889  | -0.530 | 24.933 | 1.00 | 9.07  |
| ATOM | 668 | CB  | TYR | A | 103 | 5.549  | -0.917 | 23.486 | 1.00 | 9.50  |
| ATOM | 669 | CG  | TYR | A | 103 | 4.870  | -2.239 | 23.265 | 1.00 | 12.57 |
| ATOM | 670 | CD1 | TYR | A | 103 | 5.544  | -3.435 | 23.487 | 1.00 | 12.90 |
| ATOM | 671 | CE1 | TYR | A | 103 | 4.895  | -4.640 | 23.272 | 1.00 | 20.46 |
| ATOM | 672 | CZ  | TYR | A | 103 | 3.592  | -4.680 | 22.839 | 1.00 | 22.70 |
| ATOM | 673 | OH  | TYR | A | 103 | 2.962  | -5.894 | 22.627 | 1.00 | 18.14 |
| ATOM | 674 | CE2 | TYR | A | 103 | 2.903  | -3.500 | 22.608 | 1.00 | 18.79 |
| ATOM | 675 | CD2 | TYR | A | 103 | 3.551  | -2.304 | 22.825 | 1.00 | 15.94 |

FIGURE 115

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 676 | C   | TYR | A | 103 | 6.867  | 0.630  | 24.891 | 1.00 | 18.09 |
| ATOM | 677 | O   | TYR | A | 103 | 6.457  | 1.768  | 24.641 | 1.00 | 20.48 |
| ATOM | 678 | N   | ILE | A | 104 | 8.155  | 0.358  | 25.111 | 1.00 | 15.21 |
| ATOM | 679 | CA  | ILE | A | 104 | 9.108  | 1.466  | 25.121 | 1.00 | 15.90 |
| ATOM | 680 | CB  | ILE | A | 104 | 9.608  | 1.785  | 26.545 | 1.00 | 22.38 |
| ATOM | 681 | CG1 | ILE | A | 104 | 8.496  | 1.941  | 27.585 | 1.00 | 20.69 |
| ATOM | 682 | CD1 | ILE | A | 104 | 7.599  | 3.126  | 27.276 | 1.00 | 17.88 |
| ATOM | 683 | CG2 | ILE | A | 104 | 10.476 | 3.034  | 26.538 | 1.00 | 22.81 |
| ATOM | 684 | C   | ILE | A | 104 | 10.309 | 1.146  | 24.243 | 1.00 | 17.74 |
| ATOM | 685 | O   | ILE | A | 104 | 10.911 | 0.086  | 24.357 | 1.00 | 16.43 |
| ATOM | 686 | N   | PRO | A | 105 | 10.677 | 2.062  | 23.352 | 1.00 | 17.30 |
| ATOM | 687 | CA  | PRO | A | 105 | 11.894 | 1.894  | 22.563 | 1.00 | 16.76 |
| ATOM | 688 | CB  | PRO | A | 105 | 11.837 | 3.088  | 21.592 | 1.00 | 24.69 |
| ATOM | 689 | CG  | PRO | A | 105 | 10.418 | 3.563  | 21.626 | 1.00 | 25.93 |
| ATOM | 690 | CD  | PRO | A | 105 | 9.941  | 3.295  | 23.030 | 1.00 | 21.65 |
| ATOM | 691 | C   | PRO | A | 105 | 13.174 | 2.007  | 23.372 | 1.00 | 21.81 |
| ATOM | 692 | O   | PRO | A | 105 | 13.286 | 2.726  | 24.368 | 1.00 | 21.23 |
| ATOM | 693 | N   | GLY | A | 106 | 14.205 | 1.282  | 22.935 | 1.00 | 17.97 |
| ATOM | 694 | CA  | GLY | A | 106 | 15.504 | 1.436  | 23.569 | 1.00 | 16.53 |
| ATOM | 695 | C   | GLY | A | 106 | 16.557 | 1.885  | 22.578 | 1.00 | 24.48 |
| ATOM | 696 | O   | GLY | A | 106 | 16.248 | 2.474  | 21.543 | 1.00 | 24.56 |
| ATOM | 697 | N   | ASN | A | 107 | 17.824 | 1.595  | 22.858 | 1.00 | 24.62 |
| ATOM | 698 | CA  | ASN | A | 107 | 18.889 | 2.049  | 21.971 | 1.00 | 31.26 |
| ATOM | 699 | CB  | ASN | A | 107 | 20.249 | 1.899  | 22.661 | 1.00 | 38.05 |
| ATOM | 700 | CG  | ASN | A | 107 | 20.775 | 3.221  | 23.184 | 1.00 | 50.06 |
| ATOM | 701 | OD1 | ASN | A | 107 | 20.008 | 4.143  | 23.476 | 1.00 | 66.78 |
| ATOM | 702 | ND2 | ASN | A | 107 | 22.094 | 3.313  | 23.301 | 1.00 | 52.90 |
| ATOM | 703 | C   | ASN | A | 107 | 18.917 | 1.269  | 20.663 | 1.00 | 30.81 |
| ATOM | 704 | O   | ASN | A | 107 | 19.482 | 1.767  | 19.693 | 1.00 | 28.48 |
| ATOM | 705 | N   | ASN | A | 108 | 18.329 | 0.080  | 20.679 | 1.00 | 32.22 |
| ATOM | 706 | CA  | ASN | A | 108 | 18.512 | -0.922 | 19.640 | 1.00 | 32.10 |
| ATOM | 707 | CB  | ASN | A | 108 | 19.098 | -2.184 | 20.305 | 1.00 | 37.07 |
| ATOM | 708 | CG  | ASN | A | 108 | 20.233 | -1.830 | 21.251 | 1.00 | 46.06 |
| ATOM | 709 | OD1 | ASN | A | 108 | 21.309 | -1.443 | 20.780 | 1.00 | 27.30 |
| ATOM | 710 | ND2 | ASN | A | 108 | 20.005 | -1.966 | 22.559 | 1.00 | 28.03 |
| ATOM | 711 | C   | ASN | A | 108 | 17.262 | -1.291 | 18.863 | 1.00 | 34.62 |
| ATOM | 712 | O   | ASN | A | 108 | 17.392 | -1.721 | 17.708 | 1.00 | 34.88 |
| ATOM | 713 | N   | PHE | A | 109 | 16.060 | -1.168 | 19.423 | 1.00 | 25.20 |
| ATOM | 714 | CA  | PHE | A | 109 | 14.840 | -1.500 | 18.690 | 1.00 | 22.97 |
| ATOM | 715 | CB  | PHE | A | 109 | 14.603 | -2.993 | 18.522 | 1.00 | 22.47 |
| ATOM | 716 | CG  | PHE | A | 109 | 14.885 | -3.951 | 19.661 | 1.00 | 28.29 |
| ATOM | 717 | CD1 | PHE | A | 109 | 13.849 | -4.560 | 20.357 | 1.00 | 24.27 |
| ATOM | 718 | CE1 | PHE | A | 109 | 14.113 | -5.455 | 21.391 | 1.00 | 22.67 |
| ATOM | 719 | CZ  | PHE | A | 109 | 15.414 | -5.748 | 21.750 | 1.00 | 19.40 |
| ATOM | 720 | CE2 | PHE | A | 109 | 16.451 | -5.143 | 21.061 | 1.00 | 34.44 |
| ATOM | 721 | CD2 | PHE | A | 109 | 16.183 | -4.259 | 20.033 | 1.00 | 33.01 |
| ATOM | 722 | C   | PHE | A | 109 | 13.620 | -0.886 | 19.383 | 1.00 | 19.13 |
| ATOM | 723 | O   | PHE | A | 109 | 13.686 | -0.531 | 20.559 | 1.00 | 20.41 |
| ATOM | 724 | N   | ARG | A | 110 | 12.538 | -0.787 | 18.641 | 1.00 | 16.32 |
| ATOM | 725 | CA  | ARG | A | 110 | 11.318 | -0.110 | 19.048 | 1.00 | 23.52 |
| ATOM | 726 | CB  | ARG | A | 110 | 10.342 | -0.036 | 17.853 | 1.00 | 22.40 |
| ATOM | 727 | CG  | ARG | A | 110 | 10.918 | 0.753  | 16.688 | 1.00 | 29.99 |

**FIGURE 116**



|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 728 | CD  | ARG | A | 110 | 9.987  | 1.901  | 16.317 | 1.00 | 44.00 |
| ATOM | 729 | NE  | ARG | A | 110 | 10.461 | 3.122  | 16.971 | 1.00 | 64.93 |
| ATOM | 730 | CZ  | ARG | A | 110 | 10.694 | 4.269  | 16.352 | 1.00 | 72.68 |
| ATOM | 731 | NH1 | ARG | A | 110 | 10.494 | 4.368  | 15.044 | 1.00 | 62.39 |
| ATOM | 732 | NH2 | ARG | A | 110 | 11.125 | 5.318  | 17.045 | 1.00 | 82.09 |
| ATOM | 733 | C   | ARG | A | 110 | 10.607 | -0.783 | 20.197 | 1.00 | 28.20 |
| ATOM | 734 | O   | ARG | A | 110 | 9.959  | -0.177 | 21.052 | 1.00 | 29.57 |
| ATOM | 735 | N   | ARG | A | 111 | 10.665 | -2.120 | 20.269 | 1.00 | 19.46 |
| ATOM | 736 | CA  | ARG | A | 111 | 9.868  | -2.607 | 21.432 | 1.00 | 19.03 |
| ATOM | 737 | CB  | ARG | A | 111 | 8.795  | -3.563 | 20.962 | 1.00 | 15.07 |
| ATOM | 738 | CG  | ARG | A | 111 | 7.581  | -2.905 | 20.332 | 1.00 | 22.11 |
| ATOM | 739 | CD  | ARG | A | 111 | 6.553  | -3.962 | 19.940 | 1.00 | 34.64 |
| ATOM | 740 | NE  | ARG | A | 111 | 5.295  | -3.339 | 19.524 | 1.00 | 33.18 |
| ATOM | 741 | CZ  | ARG | A | 111 | 4.166  | -4.022 | 19.393 | 1.00 | 25.21 |
| ATOM | 742 | NH1 | ARG | A | 111 | 4.172  | -5.327 | 19.654 | 1.00 | 22.23 |
| ATOM | 743 | NH2 | ARG | A | 111 | 3.074  | -3.380 | 19.012 | 1.00 | 32.75 |
| ATOM | 744 | C   | ARG | A | 111 | 10.831 | -3.241 | 22.417 | 1.00 | 17.42 |
| ATOM | 745 | O   | ARG | A | 111 | 10.720 | -4.425 | 22.726 | 1.00 | 18.84 |
| ATOM | 746 | N   | GLU | A | 112 | 11.800 | -2.432 | 22.855 | 1.00 | 12.49 |
| ATOM | 747 | CA  | GLU | A | 112 | 12.900 | -2.998 | 23.629 | 1.00 | 13.99 |
| ATOM | 748 | CB  | GLU | A | 112 | 14.070 | -2.005 | 23.581 | 1.00 | 15.59 |
| ATOM | 749 | CG  | GLU | A | 112 | 15.378 | -2.703 | 23.860 | 1.00 | 21.33 |
| ATOM | 750 | CD  | GLU | A | 112 | 16.623 | -2.023 | 23.352 | 1.00 | 27.40 |
| ATOM | 751 | OE1 | GLU | A | 112 | 17.658 | -2.284 | 23.998 | 1.00 | 26.38 |
| ATOM | 752 | OE2 | GLU | A | 112 | 16.619 | -1.264 | 22.363 | 1.00 | 25.78 |
| ATOM | 753 | C   | GLU | A | 112 | 12.516 | -3.334 | 25.062 | 1.00 | 18.95 |
| ATOM | 754 | O   | GLU | A | 112 | 13.022 | -4.273 | 25.693 | 1.00 | 14.06 |
| ATOM | 755 | N   | TYR | A | 113 | 11.576 | -2.551 | 25.570 | 1.00 | 17.52 |
| ATOM | 756 | CA  | TYR | A | 113 | 11.060 | -2.731 | 26.911 | 1.00 | 15.61 |
| ATOM | 757 | CB  | TYR | A | 113 | 11.542 | -1.629 | 27.858 | 1.00 | 17.96 |
| ATOM | 758 | CG  | TYR | A | 113 | 12.990 | -1.237 | 27.756 | 1.00 | 14.87 |
| ATOM | 759 | CD1 | TYR | A | 113 | 13.405 | -0.255 | 26.878 | 1.00 | 17.71 |
| ATOM | 760 | CE1 | TYR | A | 113 | 14.734 | 0.114  | 26.781 | 1.00 | 16.32 |
| ATOM | 761 | CZ  | TYR | A | 113 | 15.671 | -0.495 | 27.574 | 1.00 | 15.65 |
| ATOM | 762 | OH  | TYR | A | 113 | 17.002 | -0.145 | 27.493 | 1.00 | 18.69 |
| ATOM | 763 | CE2 | TYR | A | 113 | 15.289 | -1.484 | 28.467 | 1.00 | 14.44 |
| ATOM | 764 | CD2 | TYR | A | 113 | 13.959 | -1.844 | 28.553 | 1.00 | 14.04 |
| ATOM | 765 | C   | TYR | A | 113 | 9.551  | -2.702 | 26.926 | 1.00 | 9.51  |
| ATOM | 766 | O   | TYR | A | 113 | 8.855  | -2.122 | 26.096 | 1.00 | 11.17 |
| ATOM | 767 | N   | ILE | A | 114 | 9.031  | -3.382 | 27.957 | 1.00 | 12.36 |
| ATOM | 768 | CA  | ILE | A | 114 | 7.655  | -3.187 | 28.333 | 1.00 | 9.29  |
| ATOM | 769 | CB  | ILE | A | 114 | 6.831  | -4.487 | 28.322 | 1.00 | 13.67 |
| ATOM | 770 | CG1 | ILE | A | 114 | 6.425  | -4.912 | 26.904 | 1.00 | 14.89 |
| ATOM | 771 | CD1 | ILE | A | 114 | 5.910  | -6.337 | 26.844 | 1.00 | 15.51 |
| ATOM | 772 | CG2 | ILE | A | 114 | 5.623  | -4.377 | 29.232 | 1.00 | 8.31  |
| ATOM | 773 | C   | ILE | A | 114 | 7.674  | -2.598 | 29.746 | 1.00 | 16.23 |
| ATOM | 774 | O   | ILE | A | 114 | 8.249  | -3.182 | 30.662 | 1.00 | 15.28 |
| ATOM | 775 | N   | VAL | A | 115 | 7.060  | -1.438 | 29.910 | 1.00 | 14.17 |
| ATOM | 776 | CA  | VAL | A | 115 | 7.015  | -0.801 | 31.225 | 1.00 | 15.15 |
| ATOM | 777 | CB  | VAL | A | 115 | 7.294  | 0.710  | 31.084 | 1.00 | 20.35 |
| ATOM | 778 | CG1 | VAL | A | 115 | 6.761  | 1.465  | 32.288 | 1.00 | 29.43 |
| ATOM | 779 | CG2 | VAL | A | 115 | 8.792  | 0.932  | 30.901 | 1.00 | 19.15 |

FIGURE 117

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |         |        |      |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 780 | C   | VAL | A | 115 | 5.645  | -1.011  | 31.821 | 1.00 | 13.67 |
| ATOM | 781 | O   | VAL | A | 115 | 4.631  | -0.945  | 31.114 | 1.00 | 12.23 |
| ATOM | 782 | N   | THR | A | 116 | 5.556  | -1.291  | 33.122 | 1.00 | 13.19 |
| ATOM | 783 | CA  | THR | A | 116 | 4.208  | -1.553  | 33.635 | 1.00 | 12.05 |
| ATOM | 784 | CB  | THR | A | 116 | 3.828  | -3.042  | 33.478 | 1.00 | 14.77 |
| ATOM | 785 | OG1 | THR | A | 116 | 2.432  | -3.257  | 33.750 | 1.00 | 13.69 |
| ATOM | 786 | CG2 | THR | A | 116 | 4.589  | -3.936  | 34.458 | 1.00 | 17.06 |
| ATOM | 787 | C   | THR | A | 116 | 4.173  | -1.057  | 35.072 | 1.00 | 9.33  |
| ATOM | 788 | O   | THR | A | 116 | 5.221  | -0.780  | 35.652 | 1.00 | 8.64  |
| ATOM | 789 | N   | GLN | A | 117 | 2.982  | -0.942  | 35.626 | 1.00 | 10.66 |
| ATOM | 790 | CA  | GLN | A | 117 | 2.843  | -0.618  | 37.039 | 1.00 | 8.65  |
| ATOM | 791 | CB  | GLN | A | 117 | 1.384  | -0.239  | 37.297 | 1.00 | 9.54  |
| ATOM | 792 | CG  | GLN | A | 117 | 0.384  | -1.351  | 37.114 | 1.00 | 12.18 |
| ATOM | 793 | CD  | GLN | A | 117 | -1.071 | -1.010  | 37.307 | 1.00 | 19.05 |
| ATOM | 794 | OE1 | GLN | A | 117 | -1.506 | 0.143   | 37.314 | 1.00 | 13.39 |
| ATOM | 795 | NE2 | GLN | A | 117 | -1.918 | -2.025  | 37.476 | 1.00 | 9.71  |
| ATOM | 796 | C   | GLN | A | 117 | 3.215  | -1.826  | 37.895 | 1.00 | 11.64 |
| ATOM | 797 | O   | GLN | A | 117 | 3.347  | -2.918  | 37.345 | 1.00 | 15.93 |
| ATOM | 798 | N   | GLY | A | 118 | 3.356  | -1.703  | 39.207 | 1.00 | 11.16 |
| ATOM | 799 | CA  | GLY | A | 118 | 3.499  | -2.903  | 40.060 | 1.00 | 10.85 |
| ATOM | 800 | C   | GLY | A | 118 | 2.157  | -3.620  | 40.096 | 1.00 | 13.55 |
| ATOM | 801 | O   | GLY | A | 118 | 1.119  | -3.034  | 40.400 | 1.00 | 15.26 |
| ATOM | 802 | N   | PRO | A | 119 | 2.148  | -4.916  | 39.758 | 1.00 | 12.96 |
| ATOM | 803 | CA  | PRO | A | 119 | 0.901  | -5.678  | 39.674 | 1.00 | 9.13  |
| ATOM | 804 | CB  | PRO | A | 119 | 1.408  | -7.119  | 39.531 | 1.00 | 18.59 |
| ATOM | 805 | CG  | PRO | A | 119 | 2.720  | -6.964  | 38.824 | 1.00 | 19.31 |
| ATOM | 806 | CD  | PRO | A | 119 | 3.341  | -5.706  | 39.396 | 1.00 | 15.37 |
| ATOM | 807 | C   | PRO | A | 119 | 0.079  | -5.567  | 40.953 | 1.00 | 8.91  |
| ATOM | 808 | O   | PRO | A | 119 | 0.680  | -5.487  | 42.027 | 1.00 | 19.14 |
| ATOM | 809 | N   | LEU | A | 120 | -1.228 | -5.555  | 40.787 | 1.00 | 13.32 |
| ATOM | 810 | CA  | LEU | A | 120 | -2.126 | -5.581  | 41.935 | 1.00 | 15.54 |
| ATOM | 811 | CB  | LEU | A | 120 | -3.388 | -4.787  | 41.631 | 1.00 | 19.85 |
| ATOM | 812 | CG  | LEU | A | 120 | -3.158 | -3.297  | 41.331 | 1.00 | 20.01 |
| ATOM | 813 | CD1 | LEU | A | 120 | -4.225 | -2.766  | 40.392 | 1.00 | 17.81 |
| ATOM | 814 | CD2 | LEU | A | 120 | -3.135 | -2.537  | 42.646 | 1.00 | 24.41 |
| ATOM | 815 | C   | LEU | A | 120 | -2.481 | -7.038  | 42.220 | 1.00 | 19.68 |
| ATOM | 816 | O   | LEU | A | 120 | -2.257 | -7.863  | 41.327 | 1.00 | 18.35 |
| ATOM | 817 | N   | PRO | A | 121 | -3.030 | -7.304  | 43.390 | 1.00 | 24.41 |
| ATOM | 818 | CA  | PRO | A | 121 | -3.516 | -8.674  | 43.666 | 1.00 | 25.78 |
| ATOM | 819 | CB  | PRO | A | 121 | -4.280 | -8.500  | 44.981 | 1.00 | 26.53 |
| ATOM | 820 | CG  | PRO | A | 121 | -3.702 | -7.283  | 45.633 | 1.00 | 23.83 |
| ATOM | 821 | CD  | PRO | A | 121 | -3.243 | -6.377  | 44.519 | 1.00 | 22.44 |
| ATOM | 822 | C   | PRO | A | 121 | -4.419 | -9.154  | 42.533 | 1.00 | 25.28 |
| ATOM | 823 | O   | PRO | A | 121 | -4.338 | -10.302 | 42.074 | 1.00 | 26.89 |
| ATOM | 824 | N   | GLY | A | 122 | -5.292 | -8.281  | 42.027 | 1.00 | 28.95 |
| ATOM | 825 | CA  | GLY | A | 122 | -6.226 | -8.601  | 40.969 | 1.00 | 25.36 |
| ATOM | 826 | C   | GLY | A | 122 | -5.706 | -8.512  | 39.557 | 1.00 | 27.04 |
| ATOM | 827 | O   | GLY | A | 122 | -6.422 | -8.858  | 38.606 | 1.00 | 25.16 |
| ATOM | 828 | N   | THR | A | 123 | -4.472 | -8.062  | 39.322 | 1.00 | 18.42 |
| ATOM | 829 | CA  | THR | A | 123 | -3.944 | -8.084  | 37.954 | 1.00 | 17.40 |
| ATOM | 830 | CB  | THR | A | 123 | -3.607 | -6.662  | 37.448 | 1.00 | 16.82 |
| ATOM | 831 | OG1 | THR | A | 123 | -2.539 | -6.104  | 38.220 | 1.00 | 16.41 |

**FIGURE 118**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |         |        |      |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 832 | CG2 | THR | A | 123 | -4.828 | -5.762  | 37.609 | 1.00 | 13.52 |
| ATOM | 833 | C   | THR | A | 123 | -2.691 | -8.924  | 37.831 | 1.00 | 15.59 |
| ATOM | 834 | O   | THR | A | 123 | -2.040 | -8.987  | 36.787 | 1.00 | 20.37 |
| ATOM | 835 | N   | LYS | A | 124 | -2.242 | -9.614  | 38.888 | 1.00 | 15.84 |
| ATOM | 836 | CA  | LYS | A | 124 | -0.996 | -10.357 | 38.635 | 1.00 | 17.87 |
| ATOM | 837 | CB  | LYS | A | 124 | -0.395 | -10.888 | 39.928 | 1.00 | 14.86 |
| ATOM | 838 | CG  | LYS | A | 124 | -1.274 | -11.701 | 40.840 | 1.00 | 15.78 |
| ATOM | 839 | CD  | LYS | A | 124 | -0.510 | -11.950 | 42.138 | 1.00 | 23.39 |
| ATOM | 840 | CE  | LYS | A | 124 | -1.394 | -12.535 | 43.232 | 1.00 | 25.01 |
| ATOM | 841 | NZ  | LYS | A | 124 | -0.522 | -12.822 | 44.422 | 1.00 | 30.58 |
| ATOM | 842 | C   | LYS | A | 124 | -1.169 | -11.500 | 37.639 | 1.00 | 13.08 |
| ATOM | 843 | O   | LYS | A | 124 | -0.190 | -11.858 | 36.969 | 1.00 | 18.52 |
| ATOM | 844 | N   | ASP | A | 125 | -2.359 | -12.084 | 37.537 | 1.00 | 16.39 |
| ATOM | 845 | CA  | ASP | A | 125 | -2.521 | -13.172 | 36.561 | 1.00 | 18.39 |
| ATOM | 846 | CB  | ASP | A | 125 | -3.854 | -13.887 | 36.710 | 1.00 | 25.32 |
| ATOM | 847 | CG  | ASP | A | 125 | -3.975 | -14.629 | 38.028 | 1.00 | 28.44 |
| ATOM | 848 | OD1 | ASP | A | 125 | -2.925 | -14.835 | 38.666 | 1.00 | 26.58 |
| ATOM | 849 | OD2 | ASP | A | 125 | -5.108 | -14.987 | 38.393 | 1.00 | 36.95 |
| ATOM | 850 | C   | ASP | A | 125 | -2.397 | -12.588 | 35.160 | 1.00 | 17.43 |
| ATOM | 851 | O   | ASP | A | 125 | -1.848 | -13.215 | 34.260 | 1.00 | 22.46 |
| ATOM | 852 | N   | ASP | A | 126 | -2.906 | -11.376 | 35.006 | 1.00 | 18.42 |
| ATOM | 853 | CA  | ASP | A | 126 | -2.740 | -10.637 | 33.754 | 1.00 | 17.99 |
| ATOM | 854 | CB  | ASP | A | 126 | -3.494 | -9.310  | 33.841 | 1.00 | 20.62 |
| ATOM | 855 | CG  | ASP | A | 126 | -4.982 | -9.448  | 34.061 | 1.00 | 38.88 |
| ATOM | 856 | OD1 | ASP | A | 126 | -5.618 | -10.322 | 33.434 | 1.00 | 37.14 |
| ATOM | 857 | OD2 | ASP | A | 126 | -5.512 | -8.656  | 34.867 | 1.00 | 50.50 |
| ATOM | 858 | C   | ASP | A | 126 | -1.278 | -10.346 | 33.451 | 1.00 | 19.58 |
| ATOM | 859 | O   | ASP | A | 126 | -0.763 | -10.451 | 32.338 | 1.00 | 19.76 |
| ATOM | 860 | N   | PHE | A | 127 | -0.558 | -9.916  | 34.485 | 1.00 | 20.86 |
| ATOM | 861 | CA  | PHE | A | 127 | 0.860  | -9.628  | 34.340 | 1.00 | 14.49 |
| ATOM | 862 | CB  | PHE | A | 127 | 1.450  | -9.238  | 35.698 | 1.00 | 12.42 |
| ATOM | 863 | CG  | PHE | A | 127 | 2.959  | -9.103  | 35.725 | 1.00 | 16.56 |
| ATOM | 864 | CD1 | PHE | A | 127 | 3.522  | -7.877  | 35.359 | 1.00 | 14.21 |
| ATOM | 865 | CE1 | PHE | A | 127 | 4.879  | -7.705  | 35.354 | 1.00 | 16.34 |
| ATOM | 866 | CZ  | PHE | A | 127 | 5.727  | -8.740  | 35.709 | 1.00 | 23.61 |
| ATOM | 867 | CE2 | PHE | A | 127 | 5.187  | -9.955  | 36.082 | 1.00 | 17.94 |
| ATOM | 868 | CD2 | PHE | A | 127 | 3.820  | -10.126 | 36.094 | 1.00 | 10.35 |
| ATOM | 869 | C   | PHE | A | 127 | 1.581  | -10.861 | 33.812 | 1.00 | 17.74 |
| ATOM | 870 | O   | PHE | A | 127 | 2.410  | -10.836 | 32.917 | 1.00 | 13.35 |
| ATOM | 871 | N   | TRP | A | 128 | 1.311  | -12.025 | 34.435 | 1.00 | 11.40 |
| ATOM | 872 | CA  | TRP | A | 128 | 2.102  | -13.181 | 33.987 | 1.00 | 15.21 |
| ATOM | 873 | CB  | TRP | A | 128 | 1.989  | -14.340 | 34.993 | 1.00 | 10.56 |
| ATOM | 874 | CG  | TRP | A | 128 | 2.845  | -14.116 | 36.205 | 1.00 | 8.09  |
| ATOM | 875 | CD1 | TRP | A | 128 | 2.376  | -13.938 | 37.463 | 1.00 | 11.21 |
| ATOM | 876 | NE1 | TRP | A | 128 | 3.421  | -13.764 | 38.325 | 1.00 | 8.52  |
| ATOM | 877 | CE2 | TRP | A | 128 | 4.594  | -13.825 | 37.643 | 1.00 | 13.75 |
| ATOM | 878 | CD2 | TRP | A | 128 | 4.266  | -14.046 | 36.298 | 1.00 | 12.80 |
| ATOM | 879 | CE3 | TRP | A | 128 | 5.315  | -14.155 | 35.373 | 1.00 | 11.11 |
| ATOM | 880 | CZ3 | TRP | A | 128 | 6.605  | -14.034 | 35.821 | 1.00 | 11.38 |
| ATOM | 881 | CH2 | TRP | A | 128 | 6.893  | -13.810 | 37.181 | 1.00 | 16.48 |
| ATOM | 882 | CZ2 | TRP | A | 128 | 5.902  | -13.701 | 38.112 | 1.00 | 15.53 |
| ATOM | 883 | C   | TRP | A | 128 | 1.654  | -13.612 | 32.601 | 1.00 | 12.30 |

**FIGURE 119**

|      |     |     |     |   |     |        |         |        |      |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 884 | O   | TRP | A | 128 | 2.460  | -14.098 | 31.798 | 1.00 | 20.27 |
| ATOM | 885 | N   | LYS | A | 129 | 0.386  | -13.432 | 32.287 | 1.00 | 14.47 |
| ATOM | 886 | CA  | LYS | A | 129 | -0.123 | -13.666 | 30.937 | 1.00 | 19.61 |
| ATOM | 887 | CB  | LYS | A | 129 | -1.619 | -13.344 | 30.895 | 1.00 | 17.71 |
| ATOM | 888 | CG  | LYS | A | 129 | -2.234 | -13.587 | 29.519 | 1.00 | 25.76 |
| ATOM | 889 | CD  | LYS | A | 129 | -3.746 | -13.768 | 29.659 | 1.00 | 30.81 |
| ATOM | 890 | CE  | LYS | A | 129 | -4.330 | -14.309 | 28.366 | 1.00 | 42.38 |
| ATOM | 891 | NZ  | LYS | A | 129 | -5.236 | -13.325 | 27.707 | 1.00 | 64.19 |
| ATOM | 892 | C   | LYS | A | 129 | 0.600  | -12.834 | 29.884 | 1.00 | 20.15 |
| ATOM | 893 | O   | LYS | A | 129 | 0.974  | -13.321 | 28.816 | 1.00 | 19.90 |
| ATOM | 894 | N   | MET | A | 130 | 0.803  | -11.553 | 30.185 | 1.00 | 15.51 |
| ATOM | 895 | CA  | MET | A | 130 | 1.625  | -10.693 | 29.342 | 1.00 | 12.30 |
| ATOM | 896 | CB  | MET | A | 130 | 1.651  | -9.264  | 29.941 | 1.00 | 13.90 |
| ATOM | 897 | CG  | MET | A | 130 | 2.496  | -8.310  | 29.089 | 1.00 | 21.15 |
| ATOM | 898 | SD  | MET | A | 130 | 2.449  | -6.632  | 29.804 | 1.00 | 18.25 |
| ATOM | 899 | CE  | MET | A | 130 | 3.476  | -6.963  | 31.261 | 1.00 | 9.99  |
| ATOM | 900 | C   | MET | A | 130 | 3.032  | -11.212 | 29.173 | 1.00 | 12.39 |
| ATOM | 901 | O   | MET | A | 130 | 3.562  | -11.277 | 28.043 | 1.00 | 16.98 |
| ATOM | 902 | N   | VAL | A | 131 | 3.694  | -11.586 | 30.273 | 1.00 | 12.09 |
| ATOM | 903 | CA  | VAL | A | 131 | 5.070  | -12.076 | 30.234 | 1.00 | 11.97 |
| ATOM | 904 | CB  | VAL | A | 131 | 5.538  | -12.430 | 31.659 | 1.00 | 16.20 |
| ATOM | 905 | CG1 | VAL | A | 131 | 6.799  | -13.282 | 31.685 | 1.00 | 15.59 |
| ATOM | 906 | CG2 | VAL | A | 131 | 5.769  | -11.144 | 32.455 | 1.00 | 15.38 |
| ATOM | 907 | C   | VAL | A | 131 | 5.163  | -13.304 | 29.317 | 1.00 | 15.84 |
| ATOM | 908 | O   | VAL | A | 131 | 6.079  | -13.467 | 28.514 | 1.00 | 16.14 |
| ATOM | 909 | N   | TRP | A | 132 | 4.164  | -14.167 | 29.469 | 1.00 | 14.48 |
| ATOM | 910 | CA  | TRP | A | 132 | 4.080  | -15.371 | 28.632 | 1.00 | 22.42 |
| ATOM | 911 | CB  | TRP | A | 132 | 2.932  | -16.265 | 29.104 | 1.00 | 21.06 |
| ATOM | 912 | CG  | TRP | A | 132 | 2.745  | -17.494 | 28.255 | 1.00 | 22.35 |
| ATOM | 913 | CD1 | TRP | A | 132 | 1.874  | -17.689 | 27.232 | 1.00 | 23.78 |
| ATOM | 914 | NE1 | TRP | A | 132 | 2.025  | -18.958 | 26.719 | 1.00 | 33.60 |
| ATOM | 915 | CE2 | TRP | A | 132 | 3.010  | -19.603 | 27.414 | 1.00 | 33.31 |
| ATOM | 916 | CD2 | TRP | A | 132 | 3.490  | -18.709 | 28.393 | 1.00 | 28.48 |
| ATOM | 917 | CE3 | TRP | A | 132 | 4.512  | -19.117 | 29.253 | 1.00 | 28.47 |
| ATOM | 918 | CZ3 | TRP | A | 132 | 5.026  | -20.393 | 29.117 | 1.00 | 36.09 |
| ATOM | 919 | CH2 | TRP | A | 132 | 4.526  | -21.255 | 28.134 | 1.00 | 36.28 |
| ATOM | 920 | CZ2 | TRP | A | 132 | 3.528  | -20.889 | 27.277 | 1.00 | 36.96 |
| ATOM | 921 | C   | TRP | A | 132 | 3.856  | -15.027 | 27.164 | 1.00 | 20.60 |
| ATOM | 922 | O   | TRP | A | 132 | 4.646  | -15.362 | 26.287 | 1.00 | 21.95 |
| ATOM | 923 | N   | GLU | A | 133 | 2.758  | -14.324 | 26.879 | 1.00 | 25.53 |
| ATOM | 924 | CA  | GLU | A | 133 | 2.457  | -13.988 | 25.485 | 1.00 | 19.74 |
| ATOM | 925 | CB  | GLU | A | 133 | 1.135  | -13.223 | 25.431 | 1.00 | 18.87 |
| ATOM | 926 | CG  | GLU | A | 133 | -0.060 | -14.082 | 25.806 | 1.00 | 25.68 |
| ATOM | 927 | CD  | GLU | A | 133 | -1.358 | -13.302 | 25.838 | 1.00 | 29.70 |
| ATOM | 928 | OE1 | GLU | A | 133 | -1.312 | -12.052 | 25.763 | 1.00 | 30.46 |
| ATOM | 929 | OE2 | GLU | A | 133 | -2.414 | -13.968 | 25.938 | 1.00 | 36.60 |
| ATOM | 930 | C   | GLU | A | 133 | 3.539  | -13.175 | 24.804 | 1.00 | 28.51 |
| ATOM | 931 | O   | GLU | A | 133 | 3.674  | -13.293 | 23.581 | 1.00 | 21.96 |
| ATOM | 932 | N   | GLN | A | 134 | 4.290  | -12.351 | 25.538 | 1.00 | 19.31 |
| ATOM | 933 | CA  | GLN | A | 134 | 5.274  | -11.491 | 24.889 | 1.00 | 19.87 |
| ATOM | 934 | CB  | GLN | A | 134 | 5.351  | -10.130 | 25.608 | 1.00 | 17.70 |
| ATOM | 935 | CG  | GLN | A | 134 | 4.018  | -9.384  | 25.508 | 1.00 | 16.42 |

**FIGURE 120**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |         |        |      |       |
|------|-----|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 936 | CD  | GLN | A | 134 | 3.914  | -8.755  | 24.122 | 1.00 | 23.73 |
| ATOM | 937 | OE1 | GLN | A | 134 | 4.912  | -8.253  | 23.602 | 1.00 | 28.15 |
| ATOM | 938 | NE2 | GLN | A | 134 | 2.717  | -8.831  | 23.569 | 1.00 | 32.92 |
| ATOM | 939 | C   | GLN | A | 134 | 6.657  | -12.107 | 24.865 | 1.00 | 20.31 |
| ATOM | 940 | O   | GLN | A | 134 | 7.638  | -11.458 | 24.496 | 1.00 | 17.95 |
| ATOM | 941 | N   | ASN | A | 135 | 6.778  | -13.370 | 25.276 | 1.00 | 19.01 |
| ATOM | 942 | CA  | ASN | A | 135 | 8.098  | -13.993 | 25.193 | 1.00 | 21.67 |
| ATOM | 943 | CB  | ASN | A | 135 | 8.553  | -13.988 | 23.723 | 1.00 | 21.93 |
| ATOM | 944 | CG  | ASN | A | 135 | 7.716  | -14.985 | 22.931 | 1.00 | 35.97 |
| ATOM | 945 | OD1 | ASN | A | 135 | 7.987  | -16.184 | 23.006 | 1.00 | 58.93 |
| ATOM | 946 | ND2 | ASN | A | 135 | 6.729  | -14.503 | 22.186 | 1.00 | 42.17 |
| ATOM | 947 | C   | ASN | A | 135 | 9.119  | -13.307 | 26.077 | 1.00 | 19.81 |
| ATOM | 948 | O   | ASN | A | 135 | 10.309 | -13.220 | 25.769 | 1.00 | 16.12 |
| ATOM | 949 | N   | VAL | A | 136 | 8.655  | -12.799 | 27.229 | 1.00 | 20.36 |
| ATOM | 950 | CA  | VAL | A | 136 | 9.581  | -12.111 | 28.122 | 1.00 | 15.08 |
| ATOM | 951 | CB  | VAL | A | 136 | 8.778  | -11.340 | 29.200 | 1.00 | 15.13 |
| ATOM | 952 | CG1 | VAL | A | 136 | 9.745  | -10.779 | 30.232 | 1.00 | 12.04 |
| ATOM | 953 | CG2 | VAL | A | 136 | 7.926  | -10.264 | 28.538 | 1.00 | 15.49 |
| ATOM | 954 | C   | VAL | A | 136 | 10.502 | -13.092 | 28.836 | 1.00 | 14.70 |
| ATOM | 955 | O   | VAL | A | 136 | 9.982  | -14.072 | 29.366 | 1.00 | 16.57 |
| ATOM | 956 | N   | HIS | A | 137 | 11.802 | -12.874 | 28.906 | 1.00 | 14.74 |
| ATOM | 957 | CA  | HIS | A | 137 | 12.674 | -13.744 | 29.696 | 1.00 | 21.99 |
| ATOM | 958 | CB  | HIS | A | 137 | 13.779 | -14.320 | 28.813 | 1.00 | 29.85 |
| ATOM | 959 | CG  | HIS | A | 137 | 13.243 | -15.085 | 27.643 | 1.00 | 41.77 |
| ATOM | 960 | ND1 | HIS | A | 137 | 12.224 | -14.609 | 26.847 | 1.00 | 47.82 |
| ATOM | 961 | CE1 | HIS | A | 137 | 11.951 | -15.483 | 25.894 | 1.00 | 50.67 |
| ATOM | 962 | NE2 | HIS | A | 137 | 12.762 | -16.515 | 26.043 | 1.00 | 51.38 |
| ATOM | 963 | CD2 | HIS | A | 137 | 13.575 | -16.290 | 27.131 | 1.00 | 52.47 |
| ATOM | 964 | C   | HIS | A | 137 | 13.278 | -12.993 | 30.881 | 1.00 | 19.04 |
| ATOM | 965 | O   | HIS | A | 137 | 13.809 | -13.584 | 31.822 | 1.00 | 20.60 |
| ATOM | 966 | N   | ASN | A | 138 | 13.193 | -11.663 | 30.864 | 1.00 | 14.47 |
| ATOM | 967 | CA  | ASN | A | 138 | 13.841 | -10.854 | 31.884 | 1.00 | 13.33 |
| ATOM | 968 | CB  | ASN | A | 138 | 15.068 | -10.147 | 31.291 | 1.00 | 17.70 |
| ATOM | 969 | CG  | ASN | A | 138 | 16.167 | -11.101 | 30.874 | 1.00 | 22.71 |
| ATOM | 970 | OD1 | ASN | A | 138 | 16.544 | -11.199 | 29.699 | 1.00 | 22.97 |
| ATOM | 971 | ND2 | ASN | A | 138 | 16.701 | -11.826 | 31.845 | 1.00 | 11.98 |
| ATOM | 972 | C   | ASN | A | 138 | 12.881 | -9.806  | 32.455 | 1.00 | 19.07 |
| ATOM | 973 | O   | ASN | A | 138 | 12.306 | -9.048  | 31.668 | 1.00 | 14.29 |
| ATOM | 974 | N   | ILE | A | 139 | 12.750 | -9.775  | 33.771 | 1.00 | 13.58 |
| ATOM | 975 | CA  | ILE | A | 139 | 11.914 | -8.814  | 34.474 | 1.00 | 17.38 |
| ATOM | 976 | CB  | ILE | A | 139 | 10.769 | -9.506  | 35.247 | 1.00 | 14.95 |
| ATOM | 977 | CG1 | ILE | A | 139 | 9.801  | -10.303 | 34.371 | 1.00 | 16.27 |
| ATOM | 978 | CD1 | ILE | A | 139 | 8.895  | -11.256 | 35.154 | 1.00 | 11.30 |
| ATOM | 979 | CG2 | ILE | A | 139 | 10.015 | -8.481  | 36.087 | 1.00 | 10.83 |
| ATOM | 980 | C   | ILE | A | 139 | 12.749 | -7.985  | 35.446 | 1.00 | 22.75 |
| ATOM | 981 | O   | ILE | A | 139 | 13.512 | -8.536  | 36.247 | 1.00 | 19.39 |
| ATOM | 982 | N   | VAL | A | 140 | 12.624 | -6.663  | 35.401 | 1.00 | 11.65 |
| ATOM | 983 | CA  | VAL | A | 140 | 13.383 | -5.800  | 36.301 | 1.00 | 8.08  |
| ATOM | 984 | CB  | VAL | A | 140 | 14.205 | -4.745  | 35.542 | 1.00 | 17.09 |
| ATOM | 985 | CG1 | VAL | A | 140 | 14.949 | -3.802  | 36.480 | 1.00 | 11.40 |
| ATOM | 986 | CG2 | VAL | A | 140 | 15.188 | -5.436  | 34.593 | 1.00 | 15.24 |
| ATOM | 987 | C   | VAL | A | 140 | 12.387 | -5.094  | 37.211 | 1.00 | 15.07 |

**FIGURE 121**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 988  | O   | VAL | A | 140 | 11.457 | -4.455 | 36.710 | 1.00 | 14.02 |
| ATOM | 989  | N   | MET | A | 141 | 12.575 | -5.238 | 38.515 | 1.00 | 14.68 |
| ATOM | 990  | CA  | MET | A | 141 | 11.685 | -4.587 | 39.483 | 1.00 | 13.84 |
| ATOM | 991  | CB  | MET | A | 141 | 11.042 | -5.664 | 40.363 | 1.00 | 10.75 |
| ATOM | 992  | CG  | MET | A | 141 | 10.187 | -5.130 | 41.494 | 1.00 | 13.65 |
| ATOM | 993  | SD  | MET | A | 141 | 9.374  | -6.486 | 42.348 | 1.00 | 17.62 |
| ATOM | 994  | CE  | MET | A | 141 | 8.443  | -5.608 | 43.606 | 1.00 | 16.36 |
| ATOM | 995  | C   | MET | A | 141 | 12.481 | -3.580 | 40.309 | 1.00 | 15.95 |
| ATOM | 996  | O   | MET | A | 141 | 13.483 | -3.948 | 40.946 | 1.00 | 13.08 |
| ATOM | 997  | N   | VAL | A | 142 | 12.088 | -2.304 | 40.318 | 1.00 | 11.30 |
| ATOM | 998  | CA  | VAL | A | 142 | 12.946 | -1.331 | 41.013 | 1.00 | 9.46  |
| ATOM | 999  | CB  | VAL | A | 142 | 13.600 | -0.291 | 40.092 | 1.00 | 13.94 |
| ATOM | 1000 | CG1 | VAL | A | 142 | 14.741 | -0.924 | 39.288 | 1.00 | 13.37 |
| ATOM | 1001 | CG2 | VAL | A | 142 | 12.590 | 0.342  | 39.149 | 1.00 | 17.83 |
| ATOM | 1002 | C   | VAL | A | 142 | 12.140 | -0.611 | 42.099 | 1.00 | 17.41 |
| ATOM | 1003 | O   | VAL | A | 142 | 12.299 | 0.591  | 42.303 | 1.00 | 23.87 |
| ATOM | 1004 | N   | THR | A | 143 | 11.299 | -1.355 | 42.791 | 1.00 | 14.35 |
| ATOM | 1005 | CA  | THR | A | 143 | 10.552 | -0.929 | 43.977 | 1.00 | 16.41 |
| ATOM | 1006 | CB  | THR | A | 143 | 9.117  | -0.509 | 43.638 | 1.00 | 23.66 |
| ATOM | 1007 | OG1 | THR | A | 143 | 8.452  | 0.041  | 44.789 | 1.00 | 20.68 |
| ATOM | 1008 | CG2 | THR | A | 143 | 8.267  | -1.698 | 43.207 | 1.00 | 9.56  |
| ATOM | 1009 | C   | THR | A | 143 | 10.561 | -2.079 | 44.982 | 1.00 | 22.05 |
| ATOM | 1010 | O   | THR | A | 143 | 10.851 | -3.218 | 44.614 | 1.00 | 15.75 |
| ATOM | 1011 | N   | GLN | A | 144 | 10.262 | -1.792 | 46.241 | 1.00 | 15.62 |
| ATOM | 1012 | CA  | GLN | A | 144 | 9.910  | -2.851 | 47.187 | 1.00 | 19.93 |
| ATOM | 1013 | CB  | GLN | A | 144 | 10.410 | -2.626 | 48.609 | 1.00 | 17.14 |
| ATOM | 1014 | CG  | GLN | A | 144 | 11.927 | -2.605 | 48.704 | 1.00 | 20.52 |
| ATOM | 1015 | CD  | GLN | A | 144 | 12.348 | -2.080 | 50.072 | 1.00 | 35.53 |
| ATOM | 1016 | OE1 | GLN | A | 144 | 12.254 | -2.790 | 51.068 | 1.00 | 40.58 |
| ATOM | 1017 | NE2 | GLN | A | 144 | 12.801 | -0.835 | 50.111 | 1.00 | 40.58 |
| ATOM | 1018 | C   | GLN | A | 144 | 8.384  | -2.911 | 47.180 | 1.00 | 22.04 |
| ATOM | 1019 | O   | GLN | A | 144 | 7.791  | -1.911 | 46.762 | 1.00 | 16.80 |
| ATOM | 1020 | N   | CYS | A | 145 | 7.844  | -4.039 | 47.614 | 1.00 | 15.58 |
| ATOM | 1021 | CA  | CYS | A | 145 | 6.417  | -4.249 | 47.637 | 1.00 | 12.91 |
| ATOM | 1022 | CB  | CYS | A | 145 | 6.103  | -5.685 | 48.076 | 1.00 | 16.62 |
| ATOM | 1023 | SG  | CYS | A | 145 | 6.632  | -6.849 | 46.778 | 1.00 | 21.90 |
| ATOM | 1024 | C   | CYS | A | 145 | 5.740  | -3.273 | 48.598 | 1.00 | 16.44 |
| ATOM | 1025 | O   | CYS | A | 145 | 4.638  | -2.796 | 48.381 | 1.00 | 16.10 |
| ATOM | 1026 | N   | VAL | A | 146 | 6.468  | -3.025 | 49.680 | 1.00 | 17.59 |
| ATOM | 1027 | CA  | VAL | A | 146 | 5.917  | -2.095 | 50.680 | 1.00 | 20.28 |
| ATOM | 1028 | CB  | VAL | A | 146 | 5.285  | -2.784 | 51.889 | 1.00 | 22.74 |
| ATOM | 1029 | CG1 | VAL | A | 146 | 4.932  | -1.757 | 52.972 | 1.00 | 22.42 |
| ATOM | 1030 | CG2 | VAL | A | 146 | 4.037  | -3.548 | 51.478 | 1.00 | 22.17 |
| ATOM | 1031 | C   | VAL | A | 146 | 7.070  | -1.198 | 51.104 | 1.00 | 16.66 |
| ATOM | 1032 | O   | VAL | A | 146 | 8.171  | -1.704 | 51.357 | 1.00 | 18.81 |
| ATOM | 1033 | N   | GLU | A | 147 | 6.824  | 0.111  | 51.141 | 1.00 | 13.43 |
| ATOM | 1034 | CA  | GLU | A | 147 | 7.898  | 0.995  | 51.588 | 1.00 | 16.86 |
| ATOM | 1035 | CB  | GLU | A | 147 | 8.417  | 1.873  | 50.447 | 1.00 | 21.49 |
| ATOM | 1036 | CG  | GLU | A | 147 | 9.145  | 1.028  | 49.405 | 1.00 | 26.38 |
| ATOM | 1037 | CD  | GLU | A | 147 | 9.550  | 1.808  | 48.172 | 1.00 | 37.10 |
| ATOM | 1038 | OE1 | GLU | A | 147 | 9.453  | 3.051  | 48.188 | 1.00 | 32.89 |
| ATOM | 1039 | OE2 | GLU | A | 147 | 9.980  | 1.139  | 47.206 | 1.00 | 27.53 |

**FIGURE 122**

|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 1040 | C   | GLU A 147 | 7.403  | 1.850  | 52.761 | 1.00 | 19.26 |
| ATOM | 1041 | O   | GLU A 147 | 6.402  | 2.535  | 52.577 | 1.00 | 27.69 |
| ATOM | 1042 | N   | LYS A 148 | 8.115  | 1.732  | 53.874 | 1.00 | 26.96 |
| ATOM | 1043 | CA  | LYS A 148 | 7.743  | 2.395  | 55.125 | 1.00 | 26.67 |
| ATOM | 1044 | CB  | LYS A 148 | 8.105  | 3.878  | 55.092 | 1.00 | 33.37 |
| ATOM | 1045 | CG  | LYS A 148 | 9.582  | 4.143  | 55.371 | 1.00 | 42.34 |
| ATOM | 1046 | CD  | LYS A 148 | 10.220 | 4.913  | 54.226 | 1.00 | 49.37 |
| ATOM | 1047 | CE  | LYS A 148 | 11.467 | 5.651  | 54.685 | 1.00 | 56.84 |
| ATOM | 1048 | NZ  | LYS A 148 | 11.213 | 7.114  | 54.810 | 1.00 | 51.81 |
| ATOM | 1049 | C   | LYS A 148 | 6.261  | 2.210  | 55.380 | 1.00 | 29.22 |
| ATOM | 1050 | O   | LYS A 148 | 5.510  | 3.102  | 55.771 | 1.00 | 34.85 |
| ATOM | 1051 | N   | GLY A 149 | 5.788  | 0.979  | 55.133 | 1.00 | 21.30 |
| ATOM | 1052 | CA  | GLY A 149 | 4.379  | 0.765  | 55.390 | 1.00 | 23.12 |
| ATOM | 1053 | C   | GLY A 149 | 3.451  | 1.142  | 54.264 | 1.00 | 28.88 |
| ATOM | 1054 | O   | GLY A 149 | 2.288  | 0.724  | 54.322 | 1.00 | 23.12 |
| ATOM | 1055 | N   | ARG A 150 | 3.892  | 1.910  | 53.264 | 1.00 | 23.43 |
| ATOM | 1056 | CA  | ARG A 150 | 2.967  | 2.235  | 52.172 | 1.00 | 19.35 |
| ATOM | 1057 | CB  | ARG A 150 | 3.237  | 3.651  | 51.657 | 1.00 | 27.51 |
| ATOM | 1058 | CG  | ARG A 150 | 3.022  | 4.689  | 52.755 | 1.00 | 36.85 |
| ATOM | 1059 | CD  | ARG A 150 | 3.433  | 6.085  | 52.332 | 1.00 | 46.96 |
| ATOM | 1060 | NE  | ARG A 150 | 4.879  | 6.252  | 52.377 | 1.00 | 54.45 |
| ATOM | 1061 | CZ  | ARG A 150 | 5.541  | 7.218  | 52.990 | 1.00 | 55.25 |
| ATOM | 1062 | NH1 | ARG A 150 | 4.899  | 8.166  | 53.652 | 1.00 | 47.81 |
| ATOM | 1063 | NH2 | ARG A 150 | 6.868  | 7.238  | 52.944 | 1.00 | 64.89 |
| ATOM | 1064 | C   | ARG A 150 | 3.097  | 1.201  | 51.060 | 1.00 | 17.74 |
| ATOM | 1065 | O   | ARG A 150 | 4.206  | 0.894  | 50.604 | 1.00 | 20.32 |
| ATOM | 1066 | N   | VAL A 151 | 1.980  | 0.628  | 50.655 | 1.00 | 18.03 |
| ATOM | 1067 | CA  | VAL A 151 | 1.948  | -0.432 | 49.654 | 1.00 | 23.37 |
| ATOM | 1068 | CB  | VAL A 151 | 0.528  | -1.030 | 49.571 | 1.00 | 28.77 |
| ATOM | 1069 | CG1 | VAL A 151 | 0.412  | -2.015 | 48.412 | 1.00 | 18.49 |
| ATOM | 1070 | CG2 | VAL A 151 | 0.162  | -1.691 | 50.895 | 1.00 | 20.07 |
| ATOM | 1071 | C   | VAL A 151 | 2.351  | 0.114  | 48.294 | 1.00 | 20.37 |
| ATOM | 1072 | O   | VAL A 151 | 1.847  | 1.164  | 47.899 | 1.00 | 19.29 |
| ATOM | 1073 | N   | LYS A 152 | 3.209  | -0.566 | 47.557 | 1.00 | 18.81 |
| ATOM | 1074 | CA  | LYS A 152 | 3.673  | -0.055 | 46.270 | 1.00 | 16.66 |
| ATOM | 1075 | CB  | LYS A 152 | 5.157  | 0.303  | 46.308 | 1.00 | 10.31 |
| ATOM | 1076 | CG  | LYS A 152 | 5.629  | 1.240  | 47.419 | 1.00 | 16.94 |
| ATOM | 1077 | CD  | LYS A 152 | 5.089  | 2.652  | 47.170 | 1.00 | 19.08 |
| ATOM | 1078 | CE  | LYS A 152 | 5.831  | 3.663  | 48.050 | 1.00 | 16.36 |
| ATOM | 1079 | NZ  | LYS A 152 | 5.565  | 5.051  | 47.592 | 1.00 | 31.76 |
| ATOM | 1080 | C   | LYS A 152 | 3.460  | -1.111 | 45.189 | 1.00 | 18.63 |
| ATOM | 1081 | O   | LYS A 152 | 3.313  | -0.808 | 44.006 | 1.00 | 14.72 |
| ATOM | 1082 | N   | CYS A 153 | 3.472  | -2.381 | 45.605 | 1.00 | 10.99 |
| ATOM | 1083 | CA  | CYS A 153 | 3.426  | -3.447 | 44.599 | 1.00 | 14.85 |
| ATOM | 1084 | CB  | CYS A 153 | 4.777  | -3.577 | 43.886 | 1.00 | 10.33 |
| ATOM | 1085 | SG  | CYS A 153 | 4.784  | -4.845 | 42.573 | 1.00 | 15.08 |
| ATOM | 1086 | C   | CYS A 153 | 3.025  | -4.752 | 45.279 | 1.00 | 19.72 |
| ATOM | 1087 | O   | CYS A 153 | 3.429  | -5.011 | 46.409 | 1.00 | 17.06 |
| ATOM | 1088 | N   | ASP A 154 | 2.207  | -5.564 | 44.633 | 1.00 | 14.81 |
| ATOM | 1089 | CA  | ASP A 154 | 1.872  | -6.852 | 45.241 | 1.00 | 15.17 |
| ATOM | 1090 | CB  | ASP A 154 | 0.662  | -7.429 | 44.514 | 1.00 | 12.59 |
| ATOM | 1091 | CG  | ASP A 154 | 0.186  | -8.745 | 45.101 | 1.00 | 24.42 |

**FIGURE 123**

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1092 | OD1 | ASP | A | 154 | 0.232  | -9.777  | 44.397 | 1.00 | 33.37 |
| ATOM | 1093 | OD2 | ASP | A | 154 | -0.223 | -8.736  | 46.278 | 1.00 | 26.94 |
| ATOM | 1094 | C   | ASP | A | 154 | 3.083  | -7.782  | 45.165 | 1.00 | 21.36 |
| ATOM | 1095 | O   | ASP | A | 154 | 3.914  | -7.662  | 44.252 | 1.00 | 23.22 |
| ATOM | 1096 | N   | HIS | A | 155 | 3.228  | -8.717  | 46.091 | 1.00 | 15.03 |
| ATOM | 1097 | CA  | HIS | A | 155 | 4.241  | -9.766  | 46.046 | 1.00 | 19.74 |
| ATOM | 1098 | CB  | HIS | A | 155 | 4.479  | -10.390 | 47.434 | 1.00 | 18.44 |
| ATOM | 1099 | CG  | HIS | A | 155 | 5.718  | -11.249 | 47.473 | 1.00 | 16.91 |
| ATOM | 1100 | ND1 | HIS | A | 155 | 5.772  | -12.503 | 46.910 | 1.00 | 21.58 |
| ATOM | 1101 | CE1 | HIS | A | 155 | 6.975  | -13.028 | 47.088 | 1.00 | 15.22 |
| ATOM | 1102 | NE2 | HIS | A | 155 | 7.719  | -12.158 | 47.752 | 1.00 | 21.40 |
| ATOM | 1103 | CD2 | HIS | A | 155 | 6.946  | -11.046 | 47.997 | 1.00 | 13.16 |
| ATOM | 1104 | C   | HIS | A | 155 | 3.765  | -10.828 | 45.054 | 1.00 | 25.16 |
| ATOM | 1105 | O   | HIS | A | 155 | 3.222  | -11.863 | 45.434 | 1.00 | 22.33 |
| ATOM | 1106 | N   | TYR | A | 156 | 3.935  | -10.543 | 43.764 | 1.00 | 14.86 |
| ATOM | 1107 | CA  | TYR | A | 156 | 3.238  | -11.265 | 42.715 | 1.00 | 14.13 |
| ATOM | 1108 | CB  | TYR | A | 156 | 3.055  | -10.354 | 41.479 | 1.00 | 13.04 |
| ATOM | 1109 | CG  | TYR | A | 156 | 4.342  | -9.814  | 40.905 | 1.00 | 13.16 |
| ATOM | 1110 | CD1 | TYR | A | 156 | 5.071  | -10.496 | 39.932 | 1.00 | 10.49 |
| ATOM | 1111 | CE1 | TYR | A | 156 | 6.239  | -10.006 | 39.407 | 1.00 | 17.75 |
| ATOM | 1112 | CZ  | TYR | A | 156 | 6.718  | -8.786  | 39.842 | 1.00 | 15.46 |
| ATOM | 1113 | OH  | TYR | A | 156 | 7.895  | -8.286  | 39.320 | 1.00 | 14.59 |
| ATOM | 1114 | CE2 | TYR | A | 156 | 6.021  | -8.087  | 40.801 | 1.00 | 14.68 |
| ATOM | 1115 | CD2 | TYR | A | 156 | 4.843  | -8.585  | 41.331 | 1.00 | 12.40 |
| ATOM | 1116 | C   | TYR | A | 156 | 3.959  | -12.526 | 42.265 | 1.00 | 17.42 |
| ATOM | 1117 | O   | TYR | A | 156 | 3.533  | -13.067 | 41.242 | 1.00 | 15.62 |
| ATOM | 1118 | N   | TRP | A | 157 | 4.994  | -12.933 | 42.972 | 1.00 | 21.73 |
| ATOM | 1119 | CA  | TRP | A | 157 | 5.722  | -14.154 | 42.677 | 1.00 | 16.38 |
| ATOM | 1120 | CB  | TRP | A | 157 | 7.152  | -13.878 | 42.223 | 1.00 | 14.65 |
| ATOM | 1121 | CG  | TRP | A | 157 | 7.993  | -13.290 | 43.317 | 1.00 | 20.93 |
| ATOM | 1122 | CD1 | TRP | A | 157 | 8.817  | -13.924 | 44.200 | 1.00 | 19.30 |
| ATOM | 1123 | NE1 | TRP | A | 157 | 9.401  | -13.009 | 45.041 | 1.00 | 18.29 |
| ATOM | 1124 | CE2 | TRP | A | 157 | 8.956  | -11.758 | 44.703 | 1.00 | 20.37 |
| ATOM | 1125 | CD2 | TRP | A | 157 | 8.070  | -11.895 | 43.622 | 1.00 | 12.37 |
| ATOM | 1126 | CE3 | TRP | A | 157 | 7.469  | -10.759 | 43.083 | 1.00 | 15.46 |
| ATOM | 1127 | CZ3 | TRP | A | 157 | 7.772  | -9.522  | 43.635 | 1.00 | 13.34 |
| ATOM | 1128 | CH2 | TRP | A | 157 | 8.657  | -9.418  | 44.709 | 1.00 | 18.59 |
| ATOM | 1129 | CZ2 | TRP | A | 157 | 9.262  | -10.519 | 45.259 | 1.00 | 21.33 |
| ATOM | 1130 | C   | TRP | A | 157 | 5.728  | -15.029 | 43.926 | 1.00 | 30.00 |
| ATOM | 1131 | O   | TRP | A | 157 | 5.456  | -14.475 | 44.994 | 1.00 | 24.21 |
| ATOM | 1132 | N   | PRO | A | 158 | 6.007  | -16.316 | 43.798 | 1.00 | 29.81 |
| ATOM | 1133 | CA  | PRO | A | 158 | 6.016  | -17.206 | 44.965 | 1.00 | 32.16 |
| ATOM | 1134 | CB  | PRO | A | 158 | 6.531  | -18.527 | 44.371 | 1.00 | 30.44 |
| ATOM | 1135 | CG  | PRO | A | 158 | 6.069  | -18.476 | 42.946 | 1.00 | 26.74 |
| ATOM | 1136 | CD  | PRO | A | 158 | 6.307  | -17.040 | 42.542 | 1.00 | 22.30 |
| ATOM | 1137 | C   | PRO | A | 158 | 6.961  | -16.803 | 46.089 | 1.00 | 29.52 |
| ATOM | 1138 | O   | PRO | A | 158 | 8.088  | -16.362 | 45.866 | 1.00 | 43.48 |
| ATOM | 1139 | N   | ALA | A | 159 | 6.502  | -16.986 | 47.322 | 1.00 | 34.03 |
| ATOM | 1140 | CA  | ALA | A | 159 | 7.303  | -16.748 | 48.519 | 1.00 | 33.58 |
| ATOM | 1141 | CB  | ALA | A | 159 | 6.444  | -16.986 | 49.760 | 1.00 | 34.30 |
| ATOM | 1142 | C   | ALA | A | 159 | 8.547  | -17.621 | 48.576 | 1.00 | 32.85 |
| ATOM | 1143 | O   | ALA | A | 159 | 9.602  | -17.201 | 49.045 | 1.00 | 40.76 |

FIGURE 124



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1144 | N   | ASP | A | 160 | 8.427  | -18.858 | 48.101 | 1.00 | 29.96 |
| ATOM | 1145 | CA  | ASP | A | 160 | 9.520  | -19.826 | 48.164 | 1.00 | 28.99 |
| ATOM | 1146 | CB  | ASP | A | 160 | 9.468  | -20.587 | 49.485 | 1.00 | 27.85 |
| ATOM | 1147 | CG  | ASP | A | 160 | 8.150  | -21.298 | 49.727 | 1.00 | 33.73 |
| ATOM | 1148 | OD1 | ASP | A | 160 | 7.767  | -21.452 | 50.910 | 1.00 | 36.35 |
| ATOM | 1149 | OD2 | ASP | A | 160 | 7.486  | -21.709 | 48.750 | 1.00 | 38.51 |
| ATOM | 1150 | C   | ASP | A | 160 | 9.449  | -20.784 | 46.983 | 1.00 | 24.92 |
| ATOM | 1151 | O   | ASP | A | 160 | 8.857  | -20.443 | 45.951 | 1.00 | 29.16 |
| ATOM | 1152 | N   | GLN | A | 161 | 10.025 | -21.975 | 47.125 | 1.00 | 19.70 |
| ATOM | 1153 | CA  | GLN | A | 161 | 10.089 | -22.904 | 46.006 | 1.00 | 29.75 |
| ATOM | 1154 | CB  | GLN | A | 161 | 11.241 | -23.901 | 46.254 | 1.00 | 33.52 |
| ATOM | 1155 | CG  | GLN | A | 161 | 12.575 | -23.383 | 45.720 | 1.00 | 41.43 |
| ATOM | 1156 | CD  | GLN | A | 161 | 13.754 | -23.856 | 46.547 | 1.00 | 53.65 |
| ATOM | 1157 | OE1 | GLN | A | 161 | 14.390 | -24.865 | 46.229 | 1.00 | 54.16 |
| ATOM | 1158 | NE2 | GLN | A | 161 | 14.053 | -23.128 | 47.619 | 1.00 | 75.55 |
| ATOM | 1159 | C   | GLN | A | 161 | 8.798  | -23.664 | 45.760 | 1.00 | 32.87 |
| ATOM | 1160 | O   | GLN | A | 161 | 8.730  | -24.481 | 44.833 | 1.00 | 27.15 |
| ATOM | 1161 | N   | ASP | A | 162 | 7.759  | -23.443 | 46.559 | 1.00 | 32.19 |
| ATOM | 1162 | CA  | ASP | A | 162 | 6.508  | -24.162 | 46.313 | 1.00 | 25.87 |
| ATOM | 1163 | CB  | ASP | A | 162 | 5.547  | -24.078 | 47.488 | 1.00 | 27.76 |
| ATOM | 1164 | CG  | ASP | A | 162 | 5.916  | -24.971 | 48.652 | 1.00 | 40.60 |
| ATOM | 1165 | OD1 | ASP | A | 162 | 7.006  | -25.582 | 48.628 | 1.00 | 39.74 |
| ATOM | 1166 | OD2 | ASP | A | 162 | 5.099  | -25.049 | 49.598 | 1.00 | 66.88 |
| ATOM | 1167 | C   | ASP | A | 162 | 5.855  | -23.557 | 45.072 | 1.00 | 29.94 |
| ATOM | 1168 | O   | ASP | A | 162 | 5.977  | -22.348 | 44.880 | 1.00 | 36.10 |
| ATOM | 1169 | N   | SER | A | 163 | 5.201  | -24.359 | 44.249 | 1.00 | 23.42 |
| ATOM | 1170 | CA  | SER | A | 163 | 4.656  | -23.839 | 42.997 | 1.00 | 21.05 |
| ATOM | 1171 | CB  | SER | A | 163 | 4.556  | -24.994 | 41.988 | 1.00 | 26.60 |
| ATOM | 1172 | OG  | SER | A | 163 | 3.896  | -26.074 | 42.630 | 1.00 | 25.84 |
| ATOM | 1173 | C   | SER | A | 163 | 3.306  | -23.190 | 43.194 | 1.00 | 17.83 |
| ATOM | 1174 | O   | SER | A | 163 | 2.600  | -23.381 | 44.183 | 1.00 | 21.12 |
| ATOM | 1175 | N   | LEU | A | 164 | 2.909  | -22.379 | 42.208 | 1.00 | 22.53 |
| ATOM | 1176 | CA  | LEU | A | 164 | 1.618  | -21.708 | 42.296 | 1.00 | 17.81 |
| ATOM | 1177 | CB  | LEU | A | 164 | 1.770  | -20.333 | 42.942 | 1.00 | 22.42 |
| ATOM | 1178 | CG  | LEU | A | 164 | 1.717  | -20.210 | 44.457 | 1.00 | 30.71 |
| ATOM | 1179 | CD1 | LEU | A | 164 | 1.783  | -18.736 | 44.854 | 1.00 | 38.32 |
| ATOM | 1180 | CD2 | LEU | A | 164 | 0.464  | -20.862 | 45.021 | 1.00 | 31.30 |
| ATOM | 1181 | C   | LEU | A | 164 | 1.042  | -21.526 | 40.897 | 1.00 | 16.82 |
| ATOM | 1182 | O   | LEU | A | 164 | 1.843  | -21.285 | 39.990 | 1.00 | 20.87 |
| ATOM | 1183 | N   | TYR | A | 165 | -0.269 | -21.616 | 40.758 | 1.00 | 15.24 |
| ATOM | 1184 | CA  | TYR | A | 165 | -0.942 | -21.169 | 39.550 | 1.00 | 22.53 |
| ATOM | 1185 | CB  | TYR | A | 165 | -2.365 | -21.741 | 39.489 | 1.00 | 16.95 |
| ATOM | 1186 | CG  | TYR | A | 165 | -2.417 | -23.194 | 39.073 | 1.00 | 20.26 |
| ATOM | 1187 | CD1 | TYR | A | 165 | -2.541 | -24.180 | 40.038 | 1.00 | 15.27 |
| ATOM | 1188 | CE1 | TYR | A | 165 | -2.593 | -25.515 | 39.711 | 1.00 | 15.03 |
| ATOM | 1189 | CZ  | TYR | A | 165 | -2.522 | -25.882 | 38.390 | 1.00 | 19.11 |
| ATOM | 1190 | OH  | TYR | A | 165 | -2.579 | -27.227 | 38.066 | 1.00 | 25.32 |
| ATOM | 1191 | CE2 | TYR | A | 165 | -2.402 | -24.928 | 37.410 | 1.00 | 19.58 |
| ATOM | 1192 | CD2 | TYR | A | 165 | -2.348 | -23.582 | 37.740 | 1.00 | 25.42 |
| ATOM | 1193 | C   | TYR | A | 165 | -1.076 | -19.646 | 39.464 | 1.00 | 25.11 |
| ATOM | 1194 | O   | TYR | A | 165 | -1.337 | -18.969 | 40.459 | 1.00 | 19.81 |
| ATOM | 1195 | N   | TYR | A | 166 | -0.938 | -19.095 | 38.264 | 1.00 | 18.82 |

**FIGURE 125**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1196 | CA  | TYR | A | 166 | -1.373 | -17.719 | 38.014 | 1.00 | 23.86 |
| ATOM | 1197 | CB  | TYR | A | 166 | -0.202 | -16.754 | 37.949 | 1.00 | 25.11 |
| ATOM | 1198 | CG  | TYR | A | 166 | 0.652  | -16.636 | 39.182 | 1.00 | 17.66 |
| ATOM | 1199 | CD1 | TYR | A | 166 | 0.365  | -15.669 | 40.134 | 1.00 | 17.33 |
| ATOM | 1200 | CE1 | TYR | A | 166 | 1.133  | -15.541 | 41.265 | 1.00 | 20.35 |
| ATOM | 1201 | CZ  | TYR | A | 166 | 2.205  | -16.369 | 41.485 | 1.00 | 26.41 |
| ATOM | 1202 | OH  | TYR | A | 166 | 2.943  | -16.198 | 42.636 | 1.00 | 24.80 |
| ATOM | 1203 | CE2 | TYR | A | 166 | 2.521  | -17.338 | 40.561 | 1.00 | 24.56 |
| ATOM | 1204 | CD2 | TYR | A | 166 | 1.738  | -17.457 | 39.421 | 1.00 | 19.47 |
| ATOM | 1205 | C   | TYR | A | 166 | -2.168 | -17.720 | 36.706 | 1.00 | 15.43 |
| ATOM | 1206 | O   | TYR | A | 166 | -1.541 | -17.809 | 35.655 | 1.00 | 16.56 |
| ATOM | 1207 | N   | GLY | A | 167 | -3.474 | -17.641 | 36.810 | 1.00 | 17.70 |
| ATOM | 1208 | CA  | GLY | A | 167 | -4.449 | -17.953 | 35.792 | 1.00 | 24.28 |
| ATOM | 1209 | C   | GLY | A | 167 | -4.211 | -19.347 | 35.220 | 1.00 | 31.57 |
| ATOM | 1210 | O   | GLY | A | 167 | -4.329 | -20.338 | 35.943 | 1.00 | 28.31 |
| ATOM | 1211 | N   | ASP | A | 168 | -3.856 | -19.435 | 33.943 | 1.00 | 24.61 |
| ATOM | 1212 | CA  | ASP | A | 168 | -3.616 | -20.695 | 33.265 | 1.00 | 28.49 |
| ATOM | 1213 | CB  | ASP | A | 168 | -4.089 | -20.622 | 31.802 | 1.00 | 29.53 |
| ATOM | 1214 | CG  | ASP | A | 168 | -5.587 | -20.382 | 31.765 | 1.00 | 33.69 |
| ATOM | 1215 | OD1 | ASP | A | 168 | -6.283 | -21.001 | 32.589 | 1.00 | 33.30 |
| ATOM | 1216 | OD2 | ASP | A | 168 | -6.063 | -19.582 | 30.947 | 1.00 | 43.14 |
| ATOM | 1217 | C   | ASP | A | 168 | -2.152 | -21.097 | 33.273 | 1.00 | 28.68 |
| ATOM | 1218 | O   | ASP | A | 168 | -1.802 | -22.113 | 32.667 | 1.00 | 34.81 |
| ATOM | 1219 | N   | LEU | A | 169 | -1.310 | -20.309 | 33.937 | 1.00 | 22.13 |
| ATOM | 1220 | CA  | LEU | A | 169 | 0.109  | -20.623 | 33.989 | 1.00 | 18.47 |
| ATOM | 1221 | CB  | LEU | A | 169 | 0.958  | -19.356 | 33.795 | 1.00 | 21.38 |
| ATOM | 1222 | CG  | LEU | A | 169 | 0.732  | -18.594 | 32.489 | 1.00 | 25.30 |
| ATOM | 1223 | CD1 | LEU | A | 169 | 1.565  | -17.313 | 32.456 | 1.00 | 21.42 |
| ATOM | 1224 | CD2 | LEU | A | 169 | 1.043  | -19.474 | 31.290 | 1.00 | 27.51 |
| ATOM | 1225 | C   | LEU | A | 169 | 0.470  | -21.268 | 35.322 | 1.00 | 19.04 |
| ATOM | 1226 | O   | LEU | A | 169 | -0.213 | -21.003 | 36.309 | 1.00 | 21.82 |
| ATOM | 1227 | N   | ILE | A | 170 | 1.516  | -22.084 | 35.337 | 1.00 | 20.12 |
| ATOM | 1228 | CA  | ILE | A | 170 | 2.068  | -22.592 | 36.587 | 1.00 | 21.11 |
| ATOM | 1229 | CB  | ILE | A | 170 | 2.138  | -24.120 | 36.675 | 1.00 | 20.24 |
| ATOM | 1230 | CG1 | ILE | A | 170 | 0.783  | -24.795 | 36.514 | 1.00 | 27.42 |
| ATOM | 1231 | CD1 | ILE | A | 170 | 0.840  | -26.292 | 36.777 | 1.00 | 29.31 |
| ATOM | 1232 | CG2 | ILE | A | 170 | 2.804  | -24.547 | 37.980 | 1.00 | 23.61 |
| ATOM | 1233 | C   | ILE | A | 170 | 3.478  | -22.031 | 36.736 | 1.00 | 20.55 |
| ATOM | 1234 | O   | ILE | A | 170 | 4.251  | -22.062 | 35.786 | 1.00 | 28.78 |
| ATOM | 1235 | N   | LEU | A | 171 | 3.763  | -21.531 | 37.926 | 1.00 | 22.31 |
| ATOM | 1236 | CA  | LEU | A | 171 | 5.044  | -20.881 | 38.181 | 1.00 | 24.43 |
| ATOM | 1237 | CB  | LEU | A | 171 | 4.758  | -19.393 | 38.433 | 1.00 | 27.91 |
| ATOM | 1238 | CG  | LEU | A | 171 | 5.910  | -18.408 | 38.278 | 1.00 | 37.79 |
| ATOM | 1239 | CD1 | LEU | A | 171 | 5.400  | -17.017 | 37.942 | 1.00 | 44.63 |
| ATOM | 1240 | CD2 | LEU | A | 171 | 6.747  | -18.374 | 39.551 | 1.00 | 34.65 |
| ATOM | 1241 | C   | LEU | A | 171 | 5.774  | -21.519 | 39.352 | 1.00 | 19.86 |
| ATOM | 1242 | O   | LEU | A | 171 | 5.179  | -21.847 | 40.382 | 1.00 | 20.05 |
| ATOM | 1243 | N   | GLN | A | 172 | 7.077  | -21.692 | 39.203 | 1.00 | 21.32 |
| ATOM | 1244 | CA  | GLN | A | 172 | 7.936  | -22.247 | 40.234 | 1.00 | 29.54 |
| ATOM | 1245 | CB  | GLN | A | 172 | 8.315  | -23.689 | 39.862 | 1.00 | 43.33 |
| ATOM | 1246 | CG  | GLN | A | 172 | 7.514  | -24.770 | 40.555 | 1.00 | 53.47 |
| ATOM | 1247 | CD  | GLN | A | 172 | 8.301  | -26.042 | 40.814 | 1.00 | 63.05 |

**FIGURE 126**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1248 | OE1 | GLN | A | 172 | 9.068  | -26.503 | 39.964 | 1.00 | 39.02 |
| ATOM | 1249 | NE2 | GLN | A | 172 | 8.114  | -26.624 | 41.998 | 1.00 | 64.69 |
| ATOM | 1250 | C   | GLN | A | 172 | 9.211  | -21.440 | 40.411 | 1.00 | 19.61 |
| ATOM | 1251 | O   | GLN | A | 172 | 9.974  | -21.265 | 39.457 | 1.00 | 19.10 |
| ATOM | 1252 | N   | MET | A | 173 | 9.497  | -20.971 | 41.628 | 1.00 | 16.88 |
| ATOM | 1253 | CA  | MET | A | 173 | 10.792 | -20.353 | 41.863 | 1.00 | 19.35 |
| ATOM | 1254 | CB  | MET | A | 173 | 10.808 | -19.485 | 43.130 | 1.00 | 24.60 |
| ATOM | 1255 | CG  | MET | A | 173 | 12.118 | -18.710 | 43.277 | 1.00 | 27.16 |
| ATOM | 1256 | SD  | MET | A | 173 | 11.885 | -17.267 | 44.349 | 1.00 | 39.15 |
| ATOM | 1257 | CE  | MET | A | 173 | 11.807 | -18.102 | 45.934 | 1.00 | 35.39 |
| ATOM | 1258 | C   | MET | A | 173 | 11.914 | -21.384 | 42.027 | 1.00 | 24.07 |
| ATOM | 1259 | O   | MET | A | 173 | 11.953 | -22.072 | 43.043 | 1.00 | 31.47 |
| ATOM | 1260 | N   | LEU | A | 174 | 12.782 | -21.438 | 41.036 | 1.00 | 23.52 |
| ATOM | 1261 | CA  | LEU | A | 174 | 13.945 | -22.311 | 40.998 | 1.00 | 33.03 |
| ATOM | 1262 | CB  | LEU | A | 174 | 14.403 | -22.478 | 39.543 | 1.00 | 27.30 |
| ATOM | 1263 | CG  | LEU | A | 174 | 13.369 | -23.075 | 38.590 | 1.00 | 32.33 |
| ATOM | 1264 | CD1 | LEU | A | 174 | 14.023 | -23.477 | 37.276 | 1.00 | 44.31 |
| ATOM | 1265 | CD2 | LEU | A | 174 | 12.665 | -24.270 | 39.214 | 1.00 | 40.73 |
| ATOM | 1266 | C   | LEU | A | 174 | 15.096 | -21.796 | 41.841 | 1.00 | 33.13 |
| ATOM | 1267 | O   | LEU | A | 174 | 15.857 | -22.565 | 42.431 | 1.00 | 36.31 |
| ATOM | 1268 | N   | SER | A | 175 | 15.271 | -20.475 | 41.923 | 1.00 | 32.25 |
| ATOM | 1269 | CA  | SER | A | 175 | 16.386 | -19.961 | 42.712 | 1.00 | 28.55 |
| ATOM | 1270 | CB  | SER | A | 175 | 17.696 | -20.148 | 41.952 | 1.00 | 36.29 |
| ATOM | 1271 | OG  | SER | A | 175 | 17.775 | -19.299 | 40.825 | 1.00 | 30.88 |
| ATOM | 1272 | C   | SER | A | 175 | 16.199 | -18.488 | 43.069 | 1.00 | 34.24 |
| ATOM | 1273 | O   | SER | A | 175 | 15.445 | -17.778 | 42.404 | 1.00 | 23.93 |
| ATOM | 1274 | N   | GLU | A | 176 | 16.909 | -18.101 | 44.118 | 1.00 | 24.79 |
| ATOM | 1275 | CA  | GLU | A | 176 | 16.841 | -16.777 | 44.717 | 1.00 | 24.84 |
| ATOM | 1276 | CB  | GLU | A | 176 | 15.678 | -16.730 | 45.704 | 1.00 | 29.85 |
| ATOM | 1277 | CG  | GLU | A | 176 | 15.447 | -15.387 | 46.377 | 1.00 | 32.22 |
| ATOM | 1278 | CD  | GLU | A | 176 | 14.223 | -15.390 | 47.270 | 1.00 | 34.82 |
| ATOM | 1279 | OE1 | GLU | A | 176 | 14.358 | -15.795 | 48.447 | 1.00 | 50.78 |
| ATOM | 1280 | OE2 | GLU | A | 176 | 13.135 | -14.988 | 46.806 | 1.00 | 39.74 |
| ATOM | 1281 | C   | GLU | A | 176 | 18.166 | -16.441 | 45.398 | 1.00 | 35.34 |
| ATOM | 1282 | O   | GLU | A | 176 | 18.519 | -17.072 | 46.397 | 1.00 | 33.01 |
| ATOM | 1283 | N   | SER | A | 177 | 18.884 | -15.477 | 44.837 | 1.00 | 29.77 |
| ATOM | 1284 | CA  | SER | A | 177 | 20.151 | -14.997 | 45.367 | 1.00 | 25.28 |
| ATOM | 1285 | CB  | SER | A | 177 | 21.299 | -15.094 | 44.377 | 1.00 | 27.96 |
| ATOM | 1286 | OG  | SER | A | 177 | 21.253 | -16.278 | 43.606 | 1.00 | 51.47 |
| ATOM | 1287 | C   | SER | A | 177 | 20.003 | -13.547 | 45.831 | 1.00 | 30.74 |
| ATOM | 1288 | O   | SER | A | 177 | 19.856 | -12.591 | 45.070 | 1.00 | 23.11 |
| ATOM | 1289 | N   | VAL | A | 178 | 20.042 | -13.454 | 47.153 | 1.00 | 31.26 |
| ATOM | 1290 | CA  | VAL | A | 178 | 19.964 | -12.168 | 47.825 | 1.00 | 31.69 |
| ATOM | 1291 | CB  | VAL | A | 178 | 19.343 | -12.317 | 49.218 | 1.00 | 34.41 |
| ATOM | 1292 | CG1 | VAL | A | 178 | 19.192 | -10.964 | 49.903 | 1.00 | 48.17 |
| ATOM | 1293 | CG2 | VAL | A | 178 | 17.989 | -13.008 | 49.117 | 1.00 | 26.99 |
| ATOM | 1294 | C   | VAL | A | 178 | 21.367 | -11.579 | 47.885 | 1.00 | 39.05 |
| ATOM | 1295 | O   | VAL | A | 178 | 22.306 | -12.239 | 48.333 | 1.00 | 45.15 |
| ATOM | 1296 | N   | LEU | A | 179 | 21.484 | -10.351 | 47.400 | 1.00 | 29.28 |
| ATOM | 1297 | CA  | LEU | A | 179 | 22.713 | -9.567  | 47.511 | 1.00 | 24.54 |
| ATOM | 1298 | CB  | LEU | A | 179 | 23.278 | -9.294  | 46.122 | 1.00 | 27.13 |
| ATOM | 1299 | CG  | LEU | A | 179 | 23.427 | -10.559 | 45.262 | 1.00 | 39.41 |

**FIGURE 127**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1300 | CD1 | LEU | A | 179 | 23.571 | -10.210 | 43.793 | 1.00 | 56.70 |
| ATOM | 1301 | CD2 | LEU | A | 179 | 24.604 | -11.381 | 45.760 | 1.00 | 42.38 |
| ATOM | 1302 | C   | LEU | A | 179 | 22.370 | -8.317  | 48.298 | 1.00 | 32.59 |
| ATOM | 1303 | O   | LEU | A | 179 | 21.180 | -8.081  | 48.548 | 1.00 | 37.75 |
| ATOM | 1304 | N   | PRO | A | 180 | 23.330 | -7.522  | 48.737 | 1.00 | 39.11 |
| ATOM | 1305 | CA  | PRO | A | 180 | 22.960 | -6.390  | 49.597 | 1.00 | 42.52 |
| ATOM | 1306 | CB  | PRO | A | 180 | 24.299 | -5.699  | 49.872 | 1.00 | 48.91 |
| ATOM | 1307 | CG  | PRO | A | 180 | 25.323 | -6.759  | 49.636 | 1.00 | 51.16 |
| ATOM | 1308 | CD  | PRO | A | 180 | 24.778 | -7.596  | 48.511 | 1.00 | 44.82 |
| ATOM | 1309 | C   | PRO | A | 180 | 22.012 | -5.425  | 48.910 | 1.00 | 35.13 |
| ATOM | 1310 | O   | PRO | A | 180 | 21.144 | -4.829  | 49.553 | 1.00 | 43.71 |
| ATOM | 1311 | N   | GLU | A | 181 | 22.138 | -5.225  | 47.594 | 1.00 | 25.87 |
| ATOM | 1312 | CA  | GLU | A | 181 | 21.282 | -4.161  | 47.054 | 1.00 | 26.32 |
| ATOM | 1313 | CB  | GLU | A | 181 | 22.162 | -3.079  | 46.420 | 1.00 | 29.01 |
| ATOM | 1314 | CG  | GLU | A | 181 | 22.810 | -2.178  | 47.465 | 1.00 | 30.02 |
| ATOM | 1315 | CD  | GLU | A | 181 | 24.001 | -1.472  | 46.840 | 1.00 | 32.75 |
| ATOM | 1316 | OE1 | GLU | A | 181 | 24.714 | -2.135  | 46.060 | 1.00 | 55.04 |
| ATOM | 1317 | OE2 | GLU | A | 181 | 24.190 | -0.279  | 47.144 | 1.00 | 78.18 |
| ATOM | 1318 | C   | GLU | A | 181 | 20.279 | -4.658  | 46.035 | 1.00 | 19.68 |
| ATOM | 1319 | O   | GLU | A | 181 | 19.432 | -3.890  | 45.579 | 1.00 | 22.96 |
| ATOM | 1320 | N   | TRP | A | 182 | 20.393 | -5.937  | 45.683 | 1.00 | 23.62 |
| ATOM | 1321 | CA  | TRP | A | 182 | 19.378 | -6.504  | 44.799 | 1.00 | 20.73 |
| ATOM | 1322 | CB  | TRP | A | 182 | 19.626 | -6.134  | 43.344 | 1.00 | 22.35 |
| ATOM | 1323 | CG  | TRP | A | 182 | 21.019 | -6.447  | 42.864 | 1.00 | 21.68 |
| ATOM | 1324 | CD1 | TRP | A | 182 | 21.493 | -7.660  | 42.455 | 1.00 | 20.02 |
| ATOM | 1325 | NE1 | TRP | A | 182 | 22.813 | -7.552  | 42.089 | 1.00 | 24.79 |
| ATOM | 1326 | CE2 | TRP | A | 182 | 23.214 | -6.252  | 42.256 | 1.00 | 33.15 |
| ATOM | 1327 | CD2 | TRP | A | 182 | 22.107 | -5.528  | 42.743 | 1.00 | 28.28 |
| ATOM | 1328 | CE3 | TRP | A | 182 | 22.241 | -4.160  | 43.006 | 1.00 | 26.77 |
| ATOM | 1329 | CZ3 | TRP | A | 182 | 23.476 | -3.579  | 42.767 | 1.00 | 34.39 |
| ATOM | 1330 | CH2 | TRP | A | 182 | 24.560 | -4.324  | 42.281 | 1.00 | 31.42 |
| ATOM | 1331 | CZ2 | TRP | A | 182 | 24.460 | -5.664  | 42.018 | 1.00 | 30.61 |
| ATOM | 1332 | C   | TRP | A | 182 | 19.349 | -8.017  | 44.977 | 1.00 | 23.48 |
| ATOM | 1333 | O   | TRP | A | 182 | 20.281 | -8.619  | 45.513 | 1.00 | 24.37 |
| ATOM | 1334 | N   | THR | A | 183 | 18.240 | -8.569  | 44.517 | 1.00 | 20.84 |
| ATOM | 1335 | CA  | THR | A | 183 | 17.987 | -10.000 | 44.561 | 1.00 | 22.33 |
| ATOM | 1336 | CB  | THR | A | 183 | 16.773 | -10.266 | 45.471 | 1.00 | 20.04 |
| ATOM | 1337 | OG1 | THR | A | 183 | 17.130 | -9.789  | 46.776 | 1.00 | 26.68 |
| ATOM | 1338 | CG2 | THR | A | 183 | 16.466 | -11.751 | 45.577 | 1.00 | 20.82 |
| ATOM | 1339 | C   | THR | A | 183 | 17.725 | -10.538 | 43.168 | 1.00 | 26.38 |
| ATOM | 1340 | O   | THR | A | 183 | 16.949 | -9.925  | 42.429 | 1.00 | 23.46 |
| ATOM | 1341 | N   | ILE | A | 184 | 18.351 | -11.655 | 42.819 | 1.00 | 16.60 |
| ATOM | 1342 | CA  | ILE | A | 184 | 18.094 | -12.248 | 41.505 | 1.00 | 14.97 |
| ATOM | 1343 | CB  | ILE | A | 184 | 19.399 | -12.402 | 40.716 | 1.00 | 20.49 |
| ATOM | 1344 | CG1 | ILE | A | 184 | 20.113 | -11.053 | 40.565 | 1.00 | 22.48 |
| ATOM | 1345 | CD1 | ILE | A | 184 | 21.400 | -11.102 | 39.778 | 1.00 | 24.88 |
| ATOM | 1346 | CG2 | ILE | A | 184 | 19.181 | -13.048 | 39.360 | 1.00 | 15.87 |
| ATOM | 1347 | C   | ILE | A | 184 | 17.374 | -13.570 | 41.711 | 1.00 | 19.06 |
| ATOM | 1348 | O   | ILE | A | 184 | 17.874 | -14.392 | 42.481 | 1.00 | 22.71 |
| ATOM | 1349 | N   | ARG | A | 185 | 16.228 | -13.724 | 41.066 | 1.00 | 17.97 |
| ATOM | 1350 | CA  | ARG | A | 185 | 15.419 | -14.931 | 41.157 | 1.00 | 18.52 |
| ATOM | 1351 | CB  | ARG | A | 185 | 14.031 | -14.667 | 41.733 | 1.00 | 15.90 |

**FIGURE 128**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1352 | CG  | ARG | A | 185 | 14.102 | -14.003 | 43.105 | 1.00 | 20.67 |
| ATOM | 1353 | CD  | ARG | A | 185 | 12.739 | -13.580 | 43.574 | 1.00 | 23.49 |
| ATOM | 1354 | NE  | ARG | A | 185 | 12.620 | -13.167 | 44.962 | 1.00 | 21.66 |
| ATOM | 1355 | CZ  | ARG | A | 185 | 12.709 | -11.898 | 45.350 | 1.00 | 25.33 |
| ATOM | 1356 | NH1 | ARG | A | 185 | 12.934 | -10.945 | 44.455 | 1.00 | 22.07 |
| ATOM | 1357 | NH2 | ARG | A | 185 | 12.581 | -11.547 | 46.624 | 1.00 | 27.50 |
| ATOM | 1358 | C   | ARG | A | 185 | 15.285 | -15.562 | 39.776 | 1.00 | 22.74 |
| ATOM | 1359 | O   | ARG | A | 185 | 15.369 | -14.866 | 38.768 | 1.00 | 20.98 |
| ATOM | 1360 | N   | GLU | A | 186 | 15.113 | -16.874 | 39.766 | 1.00 | 23.54 |
| ATOM | 1361 | CA  | GLU | A | 186 | 14.810 | -17.562 | 38.512 | 1.00 | 27.25 |
| ATOM | 1362 | CB  | GLU | A | 186 | 15.910 | -18.545 | 38.151 | 1.00 | 26.23 |
| ATOM | 1363 | CG  | GLU | A | 186 | 16.337 | -18.573 | 36.696 | 1.00 | 29.12 |
| ATOM | 1364 | CD  | GLU | A | 186 | 17.731 | -19.181 | 36.591 | 1.00 | 39.66 |
| ATOM | 1365 | OE1 | GLU | A | 186 | 18.272 | -19.548 | 37.660 | 1.00 | 56.70 |
| ATOM | 1366 | OE2 | GLU | A | 186 | 18.262 | -19.282 | 35.470 | 1.00 | 48.51 |
| ATOM | 1367 | C   | GLU | A | 186 | 13.463 | -18.273 | 38.668 | 1.00 | 22.29 |
| ATOM | 1368 | O   | GLU | A | 186 | 13.280 | -18.945 | 39.685 | 1.00 | 18.10 |
| ATOM | 1369 | N   | PHE | A | 187 | 12.578 | -18.097 | 37.695 | 1.00 | 18.63 |
| ATOM | 1370 | CA  | PHE | A | 187 | 11.303 | -18.785 | 37.643 | 1.00 | 16.57 |
| ATOM | 1371 | CB  | PHE | A | 187 | 10.106 | -17.835 | 37.663 | 1.00 | 17.31 |
| ATOM | 1372 | CG  | PHE | A | 187 | 10.225 | -16.820 | 38.799 | 1.00 | 28.29 |
| ATOM | 1373 | CD1 | PHE | A | 187 | 10.561 | -15.507 | 38.521 | 1.00 | 35.36 |
| ATOM | 1374 | CE1 | PHE | A | 187 | 10.660 | -14.575 | 39.550 | 1.00 | 25.40 |
| ATOM | 1375 | CZ  | PHE | A | 187 | 10.448 | -14.987 | 40.849 | 1.00 | 21.30 |
| ATOM | 1376 | CE2 | PHE | A | 187 | 10.104 | -16.285 | 41.143 | 1.00 | 18.72 |
| ATOM | 1377 | CD2 | PHE | A | 187 | 9.991  | -17.207 | 40.113 | 1.00 | 25.67 |
| ATOM | 1378 | C   | PHE | A | 187 | 11.210 | -19.663 | 36.381 | 1.00 | 26.48 |
| ATOM | 1379 | O   | PHE | A | 187 | 11.754 | -19.296 | 35.347 | 1.00 | 22.46 |
| ATOM | 1380 | N   | LYS | A | 188 | 10.530 | -20.777 | 36.559 | 1.00 | 27.77 |
| ATOM | 1381 | CA  | LYS | A | 188 | 10.122 | -21.741 | 35.559 | 1.00 | 29.70 |
| ATOM | 1382 | CB  | LYS | A | 188 | 10.530 | -23.158 | 35.948 | 1.00 | 39.93 |
| ATOM | 1383 | CG  | LYS | A | 188 | 9.420  | -24.194 | 35.867 | 1.00 | 49.03 |
| ATOM | 1384 | CD  | LYS | A | 188 | 9.938  | -25.587 | 36.210 | 1.00 | 53.96 |
| ATOM | 1385 | CE  | LYS | A | 188 | 8.835  | -26.451 | 36.802 | 1.00 | 55.37 |
| ATOM | 1386 | NZ  | LYS | A | 188 | 8.767  | -27.803 | 36.178 | 1.00 | 45.26 |
| ATOM | 1387 | C   | LYS | A | 188 | 8.603  | -21.640 | 35.400 | 1.00 | 23.00 |
| ATOM | 1388 | O   | LYS | A | 188 | 7.888  | -21.828 | 36.378 | 1.00 | 26.46 |
| ATOM | 1389 | N   | ILE | A | 189 | 8.132  | -21.324 | 34.203 | 1.00 | 23.28 |
| ATOM | 1390 | CA  | ILE | A | 189 | 6.734  | -21.106 | 33.898 | 1.00 | 25.13 |
| ATOM | 1391 | CB  | ILE | A | 189 | 6.489  | -19.717 | 33.278 | 1.00 | 37.23 |
| ATOM | 1392 | CG1 | ILE | A | 189 | 6.899  | -18.538 | 34.159 | 1.00 | 42.70 |
| ATOM | 1393 | CD1 | ILE | A | 189 | 6.097  | -17.286 | 33.840 | 1.00 | 58.33 |
| ATOM | 1394 | CG2 | ILE | A | 189 | 5.029  | -19.569 | 32.866 | 1.00 | 42.16 |
| ATOM | 1395 | C   | ILE | A | 189 | 6.228  | -22.144 | 32.895 | 1.00 | 28.65 |
| ATOM | 1396 | O   | ILE | A | 189 | 6.897  | -22.279 | 31.869 | 1.00 | 28.97 |
| ATOM | 1397 | N   | CYS | A | 190 | 5.129  | -22.799 | 33.219 | 1.00 | 28.96 |
| ATOM | 1398 | CA  | CYS | A | 190 | 4.509  | -23.828 | 32.396 | 1.00 | 35.44 |
| ATOM | 1399 | CB  | CYS | A | 190 | 4.306  | -25.127 | 33.185 | 1.00 | 38.00 |
| ATOM | 1400 | SG  | CYS | A | 190 | 5.768  | -25.627 | 34.128 | 1.00 | 68.71 |
| ATOM | 1401 | C   | CYS | A | 190 | 3.178  | -23.331 | 31.836 | 1.00 | 40.13 |
| ATOM | 1402 | O   | CYS | A | 190 | 2.263  | -22.985 | 32.586 | 1.00 | 32.30 |
| ATOM | 1403 | N   | GLY | A | 191 | 3.122  | -23.308 | 30.510 | 1.00 | 37.25 |

**FIGURE 129**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |         |        |      |        |
|------|------|-----|-----------|--------|---------|--------|------|--------|
| ATOM | 1404 | CA  | GLY A 191 | 2.017  | -22.800 | 29.737 | 1.00 | 41.56  |
| ATOM | 1405 | C   | GLY A 191 | 1.357  | -23.872 | 28.890 | 1.00 | 48.56  |
| ATOM | 1406 | O   | GLY A 191 | 1.577  | -25.066 | 29.095 | 1.00 | 45.07  |
| ATOM | 1407 | N   | GLU A 192 | 0.549  | -23.428 | 27.936 | 1.00 | 54.18  |
| ATOM | 1408 | CA  | GLU A 192 | -0.200 | -24.305 | 27.048 | 1.00 | 69.22  |
| ATOM | 1409 | CB  | GLU A 192 | -1.434 | -23.566 | 26.522 | 1.00 | 74.04  |
| ATOM | 1410 | CG  | GLU A 192 | -2.761 | -24.220 | 26.866 | 1.00 | 80.18  |
| ATOM | 1411 | CD  | GLU A 192 | -3.579 | -23.505 | 27.916 | 1.00 | 81.21  |
| ATOM | 1412 | OE1 | GLU A 192 | -3.733 | -24.045 | 29.033 | 1.00 | 64.52  |
| ATOM | 1413 | OE2 | GLU A 192 | -4.092 | -22.396 | 27.649 | 1.00 | 98.21  |
| ATOM | 1414 | C   | GLU A 192 | 0.670  | -24.817 | 25.901 | 1.00 | 77.66  |
| ATOM | 1415 | O   | GLU A 192 | 0.153  | -25.106 | 24.821 | 1.00 | 91.62  |
| ATOM | 1416 | N   | GLU A 193 | 1.963  | -24.929 | 26.155 | 1.00 | 83.58  |
| ATOM | 1417 | CA  | GLU A 193 | 3.011  | -25.361 | 25.250 | 1.00 | 93.54  |
| ATOM | 1418 | CB  | GLU A 193 | 2.953  | -26.877 | 25.035 | 1.00 | 96.89  |
| ATOM | 1419 | CG  | GLU A 193 | 4.249  | -27.604 | 25.348 | 1.00 | 98.33  |
| ATOM | 1420 | CD  | GLU A 193 | 4.432  | -28.893 | 24.572 | 1.00 | 96.49  |
| ATOM | 1421 | OE1 | GLU A 193 | 3.518  | -29.278 | 23.811 | 1.00 | 93.16  |
| ATOM | 1422 | OE2 | GLU A 193 | 5.494  | -29.536 | 24.722 | 1.00 | 88.57  |
| ATOM | 1423 | C   | GLU A 193 | 2.918  | -24.636 | 23.910 | 1.00 | 99.98  |
| ATOM | 1424 | O   | GLU A 193 | 2.701  | -25.271 | 22.877 | 1.00 | 108.24 |
| ATOM | 1425 | N   | GLN A 194 | 3.077  | -23.317 | 23.931 | 1.00 | 102.55 |
| ATOM | 1426 | CA  | GLN A 194 | 2.938  | -22.499 | 22.728 | 1.00 | 105.80 |
| ATOM | 1427 | CB  | GLN A 194 | 2.358  | -21.129 | 23.088 | 1.00 | 108.21 |
| ATOM | 1428 | CG  | GLN A 194 | 0.857  | -21.133 | 23.330 | 1.00 | 106.39 |
| ATOM | 1429 | CD  | GLN A 194 | 0.501  | -21.310 | 24.793 | 1.00 | 103.56 |
| ATOM | 1430 | OE1 | GLN A 194 | 1.330  | -21.724 | 25.602 | 1.00 | 98.95  |
| ATOM | 1431 | NE2 | GLN A 194 | -0.741 | -20.994 | 25.143 | 1.00 | 99.79  |
| ATOM | 1432 | C   | GLN A 194 | 4.267  | -22.341 | 21.999 | 1.00 | 105.62 |
| ATOM | 1433 | O   | GLN A 194 | 4.998  | -23.324 | 21.847 | 1.00 | 116.12 |
| ATOM | 1434 | N   | LEU A 195 | 4.582  | -21.125 | 21.553 | 1.00 | 101.17 |
| ATOM | 1435 | CA  | LEU A 195 | 5.860  | -20.881 | 20.883 | 1.00 | 95.89  |
| ATOM | 1436 | CB  | LEU A 195 | 6.034  | -19.411 | 20.507 | 1.00 | 88.27  |
| ATOM | 1437 | CG  | LEU A 195 | 6.093  | -19.063 | 19.016 | 1.00 | 76.59  |
| ATOM | 1438 | CD1 | LEU A 195 | 6.613  | -17.648 | 18.786 | 1.00 | 35.43  |
| ATOM | 1439 | CD2 | LEU A 195 | 6.948  | -20.068 | 18.254 | 1.00 | 62.06  |
| ATOM | 1440 | C   | LEU A 195 | 7.001  | -21.372 | 21.776 | 1.00 | 95.74  |
| ATOM | 1441 | O   | LEU A 195 | 8.005  | -21.890 | 21.287 | 1.00 | 104.53 |
| ATOM | 1442 | N   | ASP A 196 | 6.831  | -21.227 | 23.085 | 1.00 | 93.29  |
| ATOM | 1443 | CA  | ASP A 196 | 7.763  | -21.771 | 24.069 | 1.00 | 89.45  |
| ATOM | 1444 | CB  | ASP A 196 | 8.450  | -20.660 | 24.857 | 1.00 | 83.52  |
| ATOM | 1445 | CG  | ASP A 196 | 7.556  | -19.912 | 25.817 | 1.00 | 71.43  |
| ATOM | 1446 | OD1 | ASP A 196 | 6.442  | -19.474 | 25.450 | 1.00 | 46.66  |
| ATOM | 1447 | OD2 | ASP A 196 | 7.964  | -19.724 | 26.984 | 1.00 | 45.20  |
| ATOM | 1448 | C   | ASP A 196 | 7.029  | -22.731 | 25.002 | 1.00 | 89.72  |
| ATOM | 1449 | O   | ASP A 196 | 5.897  | -22.456 | 25.409 | 1.00 | 82.68  |
| ATOM | 1450 | N   | ALA A 197 | 7.657  | -23.857 | 25.335 | 1.00 | 93.55  |
| ATOM | 1451 | CA  | ALA A 197 | 7.020  | -24.842 | 26.208 | 1.00 | 94.35  |
| ATOM | 1452 | CB  | ALA A 197 | 7.240  | -26.255 | 25.691 | 1.00 | 80.84  |
| ATOM | 1453 | C   | ALA A 197 | 7.520  | -24.718 | 27.644 | 1.00 | 94.80  |
| ATOM | 1454 | O   | ALA A 197 | 6.712  | -24.641 | 28.574 | 1.00 | 92.09  |
| ATOM | 1455 | N   | HIS A 198 | 8.839  | -24.700 | 27.838 | 1.00 | 92.53  |

**FIGURE 130**

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1456 | CA  | HIS | A | 198 | 9.370  | -24.519 | 29.182 | 1.00 | 88.28 |
| ATOM | 1457 | CB  | HIS | A | 198 | 10.131 | -25.748 | 29.703 | 1.00 | 89.87 |
| ATOM | 1458 | CG  | HIS | A | 198 | 10.859 | -25.377 | 30.967 | 1.00 | 91.21 |
| ATOM | 1459 | ND1 | HIS | A | 198 | 10.190 | -24.902 | 32.073 | 1.00 | 94.03 |
| ATOM | 1460 | CE1 | HIS | A | 198 | 11.057 | -24.649 | 33.038 | 1.00 | 94.08 |
| ATOM | 1461 | NE2 | HIS | A | 198 | 12.268 | -24.939 | 32.593 | 1.00 | 94.64 |
| ATOM | 1462 | CD2 | HIS | A | 198 | 12.167 | -25.392 | 31.299 | 1.00 | 92.48 |
| ATOM | 1463 | C   | HIS | A | 198 | 10.316 | -23.322 | 29.267 | 1.00 | 77.76 |
| ATOM | 1464 | O   | HIS | A | 198 | 11.500 | -23.417 | 28.954 | 1.00 | 88.55 |
| ATOM | 1465 | N   | ARG | A | 199 | 9.769  | -22.197 | 29.709 | 1.00 | 65.70 |
| ATOM | 1466 | CA  | ARG | A | 199 | 10.523 | -20.957 | 29.782 | 1.00 | 47.47 |
| ATOM | 1467 | CB  | ARG | A | 199 | 9.612  | -19.780 | 29.400 | 1.00 | 44.67 |
| ATOM | 1468 | CG  | ARG | A | 199 | 10.165 | -18.453 | 29.889 | 1.00 | 53.42 |
| ATOM | 1469 | CD  | ARG | A | 199 | 9.994  | -17.331 | 28.879 | 1.00 | 46.83 |
| ATOM | 1470 | NE  | ARG | A | 199 | 8.914  | -17.624 | 27.941 | 1.00 | 46.19 |
| ATOM | 1471 | CZ  | ARG | A | 199 | 7.852  | -16.844 | 27.777 | 1.00 | 51.98 |
| ATOM | 1472 | NH1 | ARG | A | 199 | 7.744  | -15.728 | 28.495 | 1.00 | 21.30 |
| ATOM | 1473 | NH2 | ARG | A | 199 | 6.920  | -17.196 | 26.901 | 1.00 | 32.81 |
| ATOM | 1474 | C   | ARG | A | 199 | 11.133 | -20.718 | 31.161 | 1.00 | 32.26 |
| ATOM | 1475 | O   | ARG | A | 199 | 10.541 | -21.045 | 32.190 | 1.00 | 25.30 |
| ATOM | 1476 | N   | LEU | A | 200 | 12.327 | -20.133 | 31.142 | 1.00 | 25.66 |
| ATOM | 1477 | CA  | LEU | A | 200 | 13.010 | -19.678 | 32.340 | 1.00 | 25.37 |
| ATOM | 1478 | CB  | LEU | A | 200 | 14.414 | -20.256 | 32.468 | 1.00 | 37.98 |
| ATOM | 1479 | CG  | LEU | A | 200 | 14.511 | -21.782 | 32.585 | 1.00 | 50.45 |
| ATOM | 1480 | CD1 | LEU | A | 200 | 15.956 | -22.239 | 32.447 | 1.00 | 66.02 |
| ATOM | 1481 | CD2 | LEU | A | 200 | 13.911 | -22.270 | 33.899 | 1.00 | 46.72 |
| ATOM | 1482 | C   | LEU | A | 200 | 13.058 | -18.146 | 32.323 | 1.00 | 26.91 |
| ATOM | 1483 | O   | LEU | A | 200 | 13.521 | -17.544 | 31.358 | 1.00 | 22.85 |
| ATOM | 1484 | N   | ILE | A | 201 | 12.549 | -17.552 | 33.391 | 1.00 | 23.54 |
| ATOM | 1485 | CA  | ILE | A | 201 | 12.463 | -16.102 | 33.528 | 1.00 | 16.69 |
| ATOM | 1486 | CB  | ILE | A | 201 | 11.023 | -15.688 | 33.897 | 1.00 | 18.39 |
| ATOM | 1487 | CG1 | ILE | A | 201 | 9.983  | -16.468 | 33.096 | 1.00 | 32.11 |
| ATOM | 1488 | CD1 | ILE | A | 201 | 9.613  | -15.818 | 31.788 | 1.00 | 38.11 |
| ATOM | 1489 | CG2 | ILE | A | 201 | 10.814 | -14.183 | 33.790 | 1.00 | 26.56 |
| ATOM | 1490 | C   | ILE | A | 201 | 13.394 | -15.625 | 34.626 | 1.00 | 17.67 |
| ATOM | 1491 | O   | ILE | A | 201 | 13.380 | -16.158 | 35.732 | 1.00 | 23.89 |
| ATOM | 1492 | N   | ARG | A | 202 | 14.218 | -14.617 | 34.353 | 1.00 | 16.91 |
| ATOM | 1493 | CA  | ARG | A | 202 | 15.020 | -14.076 | 35.443 | 1.00 | 13.64 |
| ATOM | 1494 | CB  | ARG | A | 202 | 16.465 | -13.807 | 35.065 | 1.00 | 20.15 |
| ATOM | 1495 | CG  | ARG | A | 202 | 17.322 | -15.053 | 34.928 | 1.00 | 33.93 |
| ATOM | 1496 | CD  | ARG | A | 202 | 18.698 | -14.896 | 35.558 | 1.00 | 44.89 |
| ATOM | 1497 | NE  | ARG | A | 202 | 19.494 | -16.112 | 35.342 | 1.00 | 57.70 |
| ATOM | 1498 | CZ  | ARG | A | 202 | 19.879 | -16.510 | 34.134 | 1.00 | 61.66 |
| ATOM | 1499 | NH1 | ARG | A | 202 | 19.549 | -15.798 | 33.063 | 1.00 | 39.90 |
| ATOM | 1500 | NH2 | ARG | A | 202 | 20.596 | -17.615 | 33.984 | 1.00 | 69.32 |
| ATOM | 1501 | C   | ARG | A | 202 | 14.351 | -12.781 | 35.905 | 1.00 | 20.61 |
| ATOM | 1502 | O   | ARG | A | 202 | 13.802 | -12.033 | 35.094 | 1.00 | 14.26 |
| ATOM | 1503 | N   | HIS | A | 203 | 14.431 | -12.604 | 37.207 | 1.00 | 18.91 |
| ATOM | 1504 | CA  | HIS | A | 203 | 13.836 | -11.436 | 37.870 | 1.00 | 18.64 |
| ATOM | 1505 | CB  | HIS | A | 203 | 12.711 | -11.896 | 38.765 | 1.00 | 13.88 |
| ATOM | 1506 | CG  | HIS | A | 203 | 11.813 | -10.917 | 39.426 | 1.00 | 22.44 |
| ATOM | 1507 | ND1 | HIS | A | 203 | 12.104 | -10.321 | 40.633 | 1.00 | 23.99 |

**FIGURE 131**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1508 | CE1 | HIS | A | 203 | 11.127 | -9.510  | 40.981 | 1.00 | 23.53 |
| ATOM | 1509 | NE2 | HIS | A | 203 | 10.189 | -9.558  | 40.046 | 1.00 | 17.09 |
| ATOM | 1510 | CD2 | HIS | A | 203 | 10.604 | -10.429 | 39.065 | 1.00 | 18.86 |
| ATOM | 1511 | C   | HIS | A | 203 | 14.961 | -10.731 | 38.626 | 1.00 | 17.56 |
| ATOM | 1512 | O   | HIS | A | 203 | 15.649 | -11.341 | 39.451 | 1.00 | 18.34 |
| ATOM | 1513 | N   | PHE | A | 204 | 15.146 | -9.457  | 38.314 | 1.00 | 15.90 |
| ATOM | 1514 | CA  | PHE | A | 204 | 16.181 | -8.621  | 38.906 | 1.00 | 15.46 |
| ATOM | 1515 | CB  | PHE | A | 204 | 17.037 | -7.984  | 37.819 | 1.00 | 15.83 |
| ATOM | 1516 | CG  | PHE | A | 204 | 17.538 | -8.995  | 36.783 | 1.00 | 15.57 |
| ATOM | 1517 | CD1 | PHE | A | 204 | 16.751 | -9.377  | 35.717 | 1.00 | 12.76 |
| ATOM | 1518 | CE1 | PHE | A | 204 | 17.208 | -10.292 | 34.785 | 1.00 | 23.10 |
| ATOM | 1519 | CZ  | PHE | A | 204 | 18.474 | -10.839 | 34.923 | 1.00 | 22.35 |
| ATOM | 1520 | CE2 | PHE | A | 204 | 19.277 | -10.461 | 35.989 | 1.00 | 21.53 |
| ATOM | 1521 | CD2 | PHE | A | 204 | 18.807 | -9.538  | 36.904 | 1.00 | 20.18 |
| ATOM | 1522 | C   | PHE | A | 204 | 15.527 | -7.556  | 39.785 | 1.00 | 20.25 |
| ATOM | 1523 | O   | PHE | A | 204 | 14.885 | -6.620  | 39.312 | 1.00 | 17.21 |
| ATOM | 1524 | N   | HIS | A | 205 | 15.672 | -7.713  | 41.097 | 1.00 | 17.28 |
| ATOM | 1525 | CA  | HIS | A | 205 | 14.949 | -6.855  | 42.035 | 1.00 | 14.35 |
| ATOM | 1526 | CB  | HIS | A | 205 | 14.203 | -7.745  | 43.021 | 1.00 | 20.27 |
| ATOM | 1527 | CG  | HIS | A | 205 | 13.221 | -7.056  | 43.900 | 1.00 | 17.93 |
| ATOM | 1528 | ND1 | HIS | A | 205 | 12.549 | -7.729  | 44.905 | 1.00 | 19.18 |
| ATOM | 1529 | CE1 | HIS | A | 205 | 11.738 | -6.874  | 45.516 | 1.00 | 22.04 |
| ATOM | 1530 | NE2 | HIS | A | 205 | 11.866 | -5.681  | 44.947 | 1.00 | 17.85 |
| ATOM | 1531 | CD2 | HIS | A | 205 | 12.788 | -5.771  | 43.928 | 1.00 | 12.88 |
| ATOM | 1532 | C   | HIS | A | 205 | 15.896 | -5.931  | 42.782 | 1.00 | 17.06 |
| ATOM | 1533 | O   | HIS | A | 205 | 16.635 | -6.400  | 43.658 | 1.00 | 21.06 |
| ATOM | 1534 | N   | TYR | A | 206 | 15.883 | -4.660  | 42.429 | 1.00 | 13.61 |
| ATOM | 1535 | CA  | TYR | A | 206 | 16.715 | -3.648  | 43.082 | 1.00 | 11.14 |
| ATOM | 1536 | CB  | TYR | A | 206 | 17.008 | -2.490  | 42.141 | 1.00 | 12.43 |
| ATOM | 1537 | CG  | TYR | A | 206 | 18.011 | -1.486  | 42.668 | 1.00 | 17.70 |
| ATOM | 1538 | CD1 | TYR | A | 206 | 19.376 | -1.745  | 42.568 | 1.00 | 14.03 |
| ATOM | 1539 | CE1 | TYR | A | 206 | 20.334 | -0.866  | 43.027 | 1.00 | 20.29 |
| ATOM | 1540 | CZ  | TYR | A | 206 | 19.892 | 0.318   | 43.602 | 1.00 | 22.75 |
| ATOM | 1541 | OH  | TYR | A | 206 | 20.839 | 1.200   | 44.070 | 1.00 | 25.15 |
| ATOM | 1542 | CE2 | TYR | A | 206 | 18.553 | 0.609   | 43.718 | 1.00 | 19.11 |
| ATOM | 1543 | CD2 | TYR | A | 206 | 17.596 | -0.287  | 43.249 | 1.00 | 18.90 |
| ATOM | 1544 | C   | TYR | A | 206 | 15.953 | -3.189  | 44.315 | 1.00 | 15.80 |
| ATOM | 1545 | O   | TYR | A | 206 | 14.828 | -2.701  | 44.188 | 1.00 | 19.33 |
| ATOM | 1546 | N   | THR | A | 207 | 16.503 | -3.371  | 45.520 | 1.00 | 16.37 |
| ATOM | 1547 | CA  | THR | A | 207 | 15.652 | -3.191  | 46.691 | 1.00 | 18.59 |
| ATOM | 1548 | CB  | THR | A | 207 | 15.789 | -4.385  | 47.669 | 1.00 | 18.47 |
| ATOM | 1549 | OG1 | THR | A | 207 | 17.175 | -4.639  | 47.895 | 1.00 | 23.23 |
| ATOM | 1550 | CG2 | THR | A | 207 | 15.217 | -5.655  | 47.056 | 1.00 | 23.19 |
| ATOM | 1551 | C   | THR | A | 207 | 15.955 | -1.923  | 47.481 | 1.00 | 23.83 |
| ATOM | 1552 | O   | THR | A | 207 | 15.371 | -1.745  | 48.556 | 1.00 | 24.21 |
| ATOM | 1553 | N   | VAL | A | 208 | 16.848 | -1.060  | 47.004 | 1.00 | 22.88 |
| ATOM | 1554 | CA  | VAL | A | 208 | 17.156 | 0.123   | 47.814 | 1.00 | 23.02 |
| ATOM | 1555 | CB  | VAL | A | 208 | 18.604 | 0.059   | 48.325 | 1.00 | 22.02 |
| ATOM | 1556 | CG1 | VAL | A | 208 | 18.747 | -1.128  | 49.276 | 1.00 | 31.63 |
| ATOM | 1557 | CG2 | VAL | A | 208 | 19.599 | -0.045  | 47.185 | 1.00 | 23.30 |
| ATOM | 1558 | C   | VAL | A | 208 | 16.951 | 1.425   | 47.059 | 1.00 | 16.29 |
| ATOM | 1559 | O   | VAL | A | 208 | 17.782 | 2.331   | 47.160 | 1.00 | 26.60 |

**FIGURE 132**



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1560 | N   | TRP | A | 209 | 15.861 | 1.525  | 46.321 | 1.00 | 14.67 |
| ATOM | 1561 | CA  | TRP | A | 209 | 15.522 | 2.734  | 45.570 | 1.00 | 21.23 |
| ATOM | 1562 | CB  | TRP | A | 209 | 15.364 | 2.460  | 44.075 | 1.00 | 23.37 |
| ATOM | 1563 | CG  | TRP | A | 209 | 15.364 | 3.656  | 43.171 | 1.00 | 17.61 |
| ATOM | 1564 | CD1 | TRP | A | 209 | 15.121 | 4.978  | 43.419 | 1.00 | 16.97 |
| ATOM | 1565 | NE1 | TRP | A | 209 | 15.236 | 5.726  | 42.271 | 1.00 | 24.39 |
| ATOM | 1566 | CE2 | TRP | A | 209 | 15.560 | 4.876  | 41.238 | 1.00 | 22.16 |
| ATOM | 1567 | CD2 | TRP | A | 209 | 15.649 | 3.568  | 41.766 | 1.00 | 16.31 |
| ATOM | 1568 | CE3 | TRP | A | 209 | 15.969 | 2.508  | 40.918 | 1.00 | 20.86 |
| ATOM | 1569 | CZ3 | TRP | A | 209 | 16.190 | 2.771  | 39.578 | 1.00 | 24.91 |
| ATOM | 1570 | CH2 | TRP | A | 209 | 16.095 | 4.077  | 39.075 | 1.00 | 20.45 |
| ATOM | 1571 | CZ2 | TRP | A | 209 | 15.785 | 5.131  | 39.888 | 1.00 | 19.42 |
| ATOM | 1572 | C   | TRP | A | 209 | 14.212 | 3.314  | 46.101 | 1.00 | 23.30 |
| ATOM | 1573 | O   | TRP | A | 209 | 13.164 | 2.827  | 45.672 | 1.00 | 25.49 |
| ATOM | 1574 | N   | PRO | A | 210 | 14.299 | 4.324  | 46.963 | 1.00 | 23.84 |
| ATOM | 1575 | CA  | PRO | A | 210 | 13.107 | 4.901  | 47.582 | 1.00 | 18.86 |
| ATOM | 1576 | CB  | PRO | A | 210 | 13.655 | 5.980  | 48.508 | 1.00 | 26.38 |
| ATOM | 1577 | CG  | PRO | A | 210 | 15.115 | 5.736  | 48.620 | 1.00 | 29.41 |
| ATOM | 1578 | CD  | PRO | A | 210 | 15.540 | 4.996  | 47.383 | 1.00 | 23.17 |
| ATOM | 1579 | C   | PRO | A | 210 | 12.199 | 5.553  | 46.536 | 1.00 | 24.85 |
| ATOM | 1580 | O   | PRO | A | 210 | 12.696 | 6.304  | 45.689 | 1.00 | 25.87 |
| ATOM | 1581 | N   | ASP | A | 211 | 10.901 | 5.271  | 46.601 | 1.00 | 19.16 |
| ATOM | 1582 | CA  | ASP | A | 211 | 9.942  | 5.886  | 45.698 | 1.00 | 23.36 |
| ATOM | 1583 | CB  | ASP | A | 211 | 8.499  | 5.590  | 46.126 | 1.00 | 25.37 |
| ATOM | 1584 | CG  | ASP | A | 211 | 7.576  | 5.865  | 44.943 | 1.00 | 24.78 |
| ATOM | 1585 | OD1 | ASP | A | 211 | 6.379  | 5.571  | 45.094 | 1.00 | 26.65 |
| ATOM | 1586 | OD2 | ASP | A | 211 | 8.078  | 6.348  | 43.899 | 1.00 | 23.48 |
| ATOM | 1587 | C   | ASP | A | 211 | 10.124 | 7.395  | 45.610 | 1.00 | 29.53 |
| ATOM | 1588 | O   | ASP | A | 211 | 10.525 | 8.061  | 46.573 | 1.00 | 32.57 |
| ATOM | 1589 | N   | HIS | A | 212 | 9.888  | 7.977  | 44.442 | 1.00 | 28.91 |
| ATOM | 1590 | CA  | HIS | A | 212 | 10.051 | 9.398  | 44.175 | 1.00 | 28.03 |
| ATOM | 1591 | CB  | HIS | A | 212 | 9.080  | 10.227 | 45.032 | 1.00 | 21.33 |
| ATOM | 1592 | CG  | HIS | A | 212 | 7.681  | 9.700  | 44.958 | 1.00 | 26.06 |
| ATOM | 1593 | ND1 | HIS | A | 212 | 6.939  | 9.760  | 43.801 | 1.00 | 23.57 |
| ATOM | 1594 | CE1 | HIS | A | 212 | 5.754  | 9.219  | 44.023 | 1.00 | 25.96 |
| ATOM | 1595 | NE2 | HIS | A | 212 | 5.703  | 8.814  | 45.279 | 1.00 | 26.25 |
| ATOM | 1596 | CD2 | HIS | A | 212 | 6.902  | 9.100  | 45.884 | 1.00 | 27.02 |
| ATOM | 1597 | C   | HIS | A | 212 | 11.460 | 9.932  | 44.425 | 1.00 | 34.91 |
| ATOM | 1598 | O   | HIS | A | 212 | 11.653 | 11.152 | 44.346 | 1.00 | 42.93 |
| ATOM | 1599 | N   | GLY | A | 213 | 12.418 | 9.071  | 44.709 | 1.00 | 25.41 |
| ATOM | 1600 | CA  | GLY | A | 213 | 13.772 | 9.392  | 45.079 | 1.00 | 25.24 |
| ATOM | 1601 | C   | GLY | A | 213 | 14.771 | 8.747  | 44.143 | 1.00 | 27.01 |
| ATOM | 1602 | O   | GLY | A | 213 | 14.471 | 8.336  | 43.027 | 1.00 | 22.02 |
| ATOM | 1603 | N   | VAL | A | 214 | 16.012 | 8.697  | 44.602 | 1.00 | 26.65 |
| ATOM | 1604 | CA  | VAL | A | 214 | 17.102 | 8.144  | 43.810 | 1.00 | 31.35 |
| ATOM | 1605 | CB  | VAL | A | 214 | 17.945 | 9.250  | 43.163 | 1.00 | 35.53 |
| ATOM | 1606 | CG1 | VAL | A | 214 | 17.091 | 10.182 | 42.307 | 1.00 | 27.84 |
| ATOM | 1607 | CG2 | VAL | A | 214 | 18.668 | 10.055 | 44.234 | 1.00 | 40.38 |
| ATOM | 1608 | C   | VAL | A | 214 | 17.953 | 7.295  | 44.742 | 1.00 | 28.56 |
| ATOM | 1609 | O   | VAL | A | 214 | 17.887 | 7.492  | 45.959 | 1.00 | 28.51 |
| ATOM | 1610 | N   | PRO | A | 215 | 18.720 | 6.349  | 44.228 | 1.00 | 23.57 |
| ATOM | 1611 | CA  | PRO | A | 215 | 19.542 | 5.511  | 45.116 | 1.00 | 29.45 |

**FIGURE 133**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1612 | CB  | PRO | A | 215 | 20.192 | 4.526  | 44.146 | 1.00 | 29.52 |
| ATOM | 1613 | CG  | PRO | A | 215 | 19.235 | 4.515  | 42.984 | 1.00 | 28.93 |
| ATOM | 1614 | CD  | PRO | A | 215 | 18.865 | 5.974  | 42.820 | 1.00 | 23.13 |
| ATOM | 1615 | C   | PRO | A | 215 | 20.601 | 6.338  | 45.842 | 1.00 | 35.63 |
| ATOM | 1616 | O   | PRO | A | 215 | 20.990 | 7.415  | 45.396 | 1.00 | 30.87 |
| ATOM | 1617 | N   | GLU | A | 216 | 21.073 | 5.828  | 46.972 | 1.00 | 35.49 |
| ATOM | 1618 | CA  | GLU | A | 216 | 22.063 | 6.538  | 47.780 | 1.00 | 35.03 |
| ATOM | 1619 | CB  | GLU | A | 216 | 22.254 | 5.768  | 49.090 | 1.00 | 36.48 |
| ATOM | 1620 | CG  | GLU | A | 216 | 23.661 | 5.715  | 49.649 | 1.00 | 52.93 |
| ATOM | 1621 | CD  | GLU | A | 216 | 23.844 | 4.606  | 50.672 | 1.00 | 63.63 |
| ATOM | 1622 | OE1 | GLU | A | 216 | 24.879 | 3.902  | 50.618 | 1.00 | 59.31 |
| ATOM | 1623 | OE2 | GLU | A | 216 | 22.952 | 4.437  | 51.532 | 1.00 | 69.52 |
| ATOM | 1624 | C   | GLU | A | 216 | 23.368 | 6.751  | 47.032 | 1.00 | 33.10 |
| ATOM | 1625 | O   | GLU | A | 216 | 24.121 | 7.675  | 47.370 | 1.00 | 39.10 |
| ATOM | 1626 | N   | THR | A | 217 | 23.711 | 5.964  | 46.014 | 1.00 | 32.88 |
| ATOM | 1627 | CA  | THR | A | 217 | 24.924 | 6.230  | 45.242 | 1.00 | 34.43 |
| ATOM | 1628 | CB  | THR | A | 217 | 26.135 | 5.360  | 45.635 | 1.00 | 41.56 |
| ATOM | 1629 | OG1 | THR | A | 217 | 25.910 | 4.010  | 45.183 | 1.00 | 31.22 |
| ATOM | 1630 | CG2 | THR | A | 217 | 26.341 | 5.329  | 47.138 | 1.00 | 44.45 |
| ATOM | 1631 | C   | THR | A | 217 | 24.711 | 5.979  | 43.748 | 1.00 | 30.56 |
| ATOM | 1632 | O   | THR | A | 217 | 23.787 | 5.258  | 43.382 | 1.00 | 25.88 |
| ATOM | 1633 | N   | THR | A | 218 | 25.578 | 6.530  | 42.901 | 1.00 | 26.73 |
| ATOM | 1634 | CA  | THR | A | 218 | 25.494 | 6.239  | 41.469 | 1.00 | 30.02 |
| ATOM | 1635 | CB  | THR | A | 218 | 26.251 | 7.270  | 40.615 | 1.00 | 29.46 |
| ATOM | 1636 | OG1 | THR | A | 218 | 27.594 | 7.382  | 41.105 | 1.00 | 27.79 |
| ATOM | 1637 | CG2 | THR | A | 218 | 25.616 | 8.644  | 40.740 | 1.00 | 30.31 |
| ATOM | 1638 | C   | THR | A | 218 | 26.045 | 4.846  | 41.171 | 1.00 | 27.66 |
| ATOM | 1639 | O   | THR | A | 218 | 25.499 | 4.105  | 40.348 | 1.00 | 23.92 |
| ATOM | 1640 | N   | GLN | A | 219 | 27.123 | 4.478  | 41.848 | 1.00 | 26.54 |
| ATOM | 1641 | CA  | GLN | A | 219 | 27.764 | 3.182  | 41.661 | 1.00 | 25.35 |
| ATOM | 1642 | CB  | GLN | A | 219 | 28.845 | 2.982  | 42.729 | 1.00 | 35.12 |
| ATOM | 1643 | CG  | GLN | A | 219 | 30.230 | 3.445  | 42.313 | 1.00 | 50.76 |
| ATOM | 1644 | CD  | GLN | A | 219 | 31.311 | 2.472  | 42.754 | 1.00 | 70.22 |
| ATOM | 1645 | OE1 | GLN | A | 219 | 31.350 | 1.331  | 42.286 | 1.00 | 92.23 |
| ATOM | 1646 | NE2 | GLN | A | 219 | 32.187 | 2.921  | 43.650 | 1.00 | 63.32 |
| ATOM | 1647 | C   | GLN | A | 219 | 26.783 | 2.013  | 41.730 | 1.00 | 26.20 |
| ATOM | 1648 | O   | GLN | A | 219 | 26.802 | 1.112  | 40.897 | 1.00 | 29.61 |
| ATOM | 1649 | N   | SER | A | 220 | 25.929 | 2.027  | 42.746 | 1.00 | 26.43 |
| ATOM | 1650 | CA  | SER | A | 220 | 24.978 | 0.956  | 42.997 | 1.00 | 31.59 |
| ATOM | 1651 | CB  | SER | A | 220 | 24.116 | 1.337  | 44.205 | 1.00 | 38.90 |
| ATOM | 1652 | OG  | SER | A | 220 | 23.043 | 0.429  | 44.379 | 1.00 | 33.12 |
| ATOM | 1653 | C   | SER | A | 220 | 24.097 | 0.682  | 41.788 | 1.00 | 31.15 |
| ATOM | 1654 | O   | SER | A | 220 | 23.995 | -0.428 | 41.264 | 1.00 | 22.82 |
| ATOM | 1655 | N   | LEU | A | 221 | 23.421 | 1.736  | 41.316 | 1.00 | 26.37 |
| ATOM | 1656 | CA  | LEU | A | 221 | 22.527 | 1.511  | 40.181 | 1.00 | 22.50 |
| ATOM | 1657 | CB  | LEU | A | 221 | 21.564 | 2.696  | 40.002 | 1.00 | 25.48 |
| ATOM | 1658 | CG  | LEU | A | 221 | 20.346 | 2.374  | 39.125 | 1.00 | 27.75 |
| ATOM | 1659 | CD1 | LEU | A | 221 | 19.596 | 1.169  | 39.683 | 1.00 | 24.04 |
| ATOM | 1660 | CD2 | LEU | A | 221 | 19.428 | 3.572  | 39.007 | 1.00 | 26.75 |
| ATOM | 1661 | C   | LEU | A | 221 | 23.311 | 1.255  | 38.907 | 1.00 | 16.37 |
| ATOM | 1662 | O   | LEU | A | 221 | 22.870 | 0.452  | 38.078 | 1.00 | 25.76 |
| ATOM | 1663 | N   | ILE | A | 222 | 24.462 | 1.917  | 38.728 | 1.00 | 17.23 |

**FIGURE 134**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1664 | CA  | ILE | A | 222 | 25.230 | 1.662  | 37.507 | 1.00 | 21.02 |
| ATOM | 1665 | CB  | ILE | A | 222 | 26.510 | 2.506  | 37.436 | 1.00 | 23.08 |
| ATOM | 1666 | CG1 | ILE | A | 222 | 26.245 | 3.966  | 37.060 | 1.00 | 23.12 |
| ATOM | 1667 | CD1 | ILE | A | 222 | 27.289 | 4.943  | 37.546 | 1.00 | 25.12 |
| ATOM | 1668 | CG2 | ILE | A | 222 | 27.498 | 1.864  | 36.473 | 1.00 | 26.15 |
| ATOM | 1669 | C   | ILE | A | 222 | 25.573 | 0.179  | 37.422 | 1.00 | 20.38 |
| ATOM | 1670 | O   | ILE | A | 222 | 25.462 | -0.473 | 36.385 | 1.00 | 18.34 |
| ATOM | 1671 | N   | GLN | A | 223 | 26.005 | -0.362 | 38.558 | 1.00 | 24.24 |
| ATOM | 1672 | CA  | GLN | A | 223 | 26.401 | -1.763 | 38.598 | 1.00 | 23.96 |
| ATOM | 1673 | CB  | GLN | A | 223 | 27.058 | -2.162 | 39.919 | 1.00 | 26.95 |
| ATOM | 1674 | CG  | GLN | A | 223 | 28.327 | -1.426 | 40.293 | 1.00 | 37.08 |
| ATOM | 1675 | CD  | GLN | A | 223 | 29.119 | -0.836 | 39.150 | 1.00 | 56.97 |
| ATOM | 1676 | OE1 | GLN | A | 223 | 29.337 | -1.473 | 38.116 | 1.00 | 84.38 |
| ATOM | 1677 | NE2 | GLN | A | 223 | 29.581 | 0.404  | 39.315 | 1.00 | 54.63 |
| ATOM | 1678 | C   | GLN | A | 223 | 25.163 | -2.627 | 38.391 | 1.00 | 24.09 |
| ATOM | 1679 | O   | GLN | A | 223 | 25.262 | -3.654 | 37.737 | 1.00 | 19.87 |
| ATOM | 1680 | N   | PHE | A | 224 | 24.017 | -2.212 | 38.943 | 1.00 | 20.92 |
| ATOM | 1681 | CA  | PHE | A | 224 | 22.831 | -3.055 | 38.717 | 1.00 | 22.52 |
| ATOM | 1682 | CB  | PHE | A | 224 | 21.658 | -2.527 | 39.529 | 1.00 | 21.20 |
| ATOM | 1683 | CG  | PHE | A | 224 | 20.330 | -3.222 | 39.302 | 1.00 | 23.79 |
| ATOM | 1684 | CD1 | PHE | A | 224 | 20.105 | -4.505 | 39.792 | 1.00 | 21.63 |
| ATOM | 1685 | CE1 | PHE | A | 224 | 18.881 | -5.123 | 39.606 | 1.00 | 15.71 |
| ATOM | 1686 | CZ  | PHE | A | 224 | 17.867 | -4.481 | 38.919 | 1.00 | 16.76 |
| ATOM | 1687 | CE2 | PHE | A | 224 | 18.074 | -3.204 | 38.415 | 1.00 | 13.56 |
| ATOM | 1688 | CD2 | PHE | A | 224 | 19.306 | -2.589 | 38.609 | 1.00 | 16.88 |
| ATOM | 1689 | C   | PHE | A | 224 | 22.477 | -3.104 | 37.240 | 1.00 | 26.00 |
| ATOM | 1690 | O   | PHE | A | 224 | 22.266 | -4.142 | 36.617 | 1.00 | 17.57 |
| ATOM | 1691 | N   | VAL | A | 225 | 22.406 | -1.916 | 36.636 | 1.00 | 17.86 |
| ATOM | 1692 | CA  | VAL | A | 225 | 22.097 | -1.855 | 35.214 | 1.00 | 14.81 |
| ATOM | 1693 | CB  | VAL | A | 225 | 22.100 | -0.383 | 34.764 | 1.00 | 15.04 |
| ATOM | 1694 | CG1 | VAL | A | 225 | 22.090 | -0.273 | 33.250 | 1.00 | 17.94 |
| ATOM | 1695 | CG2 | VAL | A | 225 | 20.903 | 0.328  | 35.391 | 1.00 | 19.94 |
| ATOM | 1696 | C   | VAL | A | 225 | 23.068 | -2.668 | 34.378 | 1.00 | 17.19 |
| ATOM | 1697 | O   | VAL | A | 225 | 22.674 | -3.427 | 33.481 | 1.00 | 19.92 |
| ATOM | 1698 | N   | ARG | A | 226 | 24.371 | -2.550 | 34.632 | 1.00 | 18.63 |
| ATOM | 1699 | CA  | ARG | A | 226 | 25.295 | -3.342 | 33.809 | 1.00 | 24.02 |
| ATOM | 1700 | CB  | ARG | A | 226 | 26.735 | -2.935 | 34.122 | 1.00 | 26.46 |
| ATOM | 1701 | CG  | ARG | A | 226 | 27.107 | -1.562 | 33.582 | 1.00 | 23.91 |
| ATOM | 1702 | CD  | ARG | A | 226 | 28.568 | -1.275 | 33.905 | 1.00 | 30.68 |
| ATOM | 1703 | NE  | ARG | A | 226 | 28.977 | 0.040  | 33.425 | 1.00 | 37.38 |
| ATOM | 1704 | CZ  | ARG | A | 226 | 29.848 | 0.828  | 34.046 | 1.00 | 45.40 |
| ATOM | 1705 | NH1 | ARG | A | 226 | 30.416 | 0.454  | 35.185 | 1.00 | 41.82 |
| ATOM | 1706 | NH2 | ARG | A | 226 | 30.154 | 2.009  | 33.522 | 1.00 | 45.68 |
| ATOM | 1707 | C   | ARG | A | 226 | 25.094 | -4.836 | 34.022 | 1.00 | 22.36 |
| ATOM | 1708 | O   | ARG | A | 226 | 25.220 | -5.649 | 33.106 | 1.00 | 24.97 |
| ATOM | 1709 | N   | THR | A | 227 | 24.762 | -5.258 | 35.243 | 1.00 | 21.54 |
| ATOM | 1710 | CA  | THR | A | 227 | 24.427 | -6.660 | 35.455 | 1.00 | 21.82 |
| ATOM | 1711 | CB  | THR | A | 227 | 24.206 | -6.945 | 36.957 | 1.00 | 29.96 |
| ATOM | 1712 | OG1 | THR | A | 227 | 25.358 | -6.463 | 37.648 | 1.00 | 28.79 |
| ATOM | 1713 | CG2 | THR | A | 227 | 24.081 | -8.437 | 37.182 | 1.00 | 29.12 |
| ATOM | 1714 | C   | THR | A | 227 | 23.182 | -7.107 | 34.713 | 1.00 | 19.03 |
| ATOM | 1715 | O   | THR | A | 227 | 23.188 | -8.158 | 34.074 | 1.00 | 26.29 |

**FIGURE 135**

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1716 | N   | VAL | A | 228 | 22.097 | -6.336  | 34.778 | 1.00 | 17.49 |
| ATOM | 1717 | CA  | VAL | A | 228 | 20.926 | -6.679  | 33.967 | 1.00 | 17.38 |
| ATOM | 1718 | CB  | VAL | A | 228 | 19.784 | -5.686  | 34.259 | 1.00 | 18.18 |
| ATOM | 1719 | CG1 | VAL | A | 228 | 18.550 | -5.978  | 33.411 | 1.00 | 19.51 |
| ATOM | 1720 | CG2 | VAL | A | 228 | 19.437 | -5.770  | 35.741 | 1.00 | 15.24 |
| ATOM | 1721 | C   | VAL | A | 228 | 21.238 | -6.711  | 32.477 | 1.00 | 17.43 |
| ATOM | 1722 | O   | VAL | A | 228 | 20.849 | -7.647  | 31.766 | 1.00 | 19.11 |
| ATOM | 1723 | N   | ARG | A | 229 | 21.943 | -5.703  | 31.972 | 1.00 | 17.01 |
| ATOM | 1724 | CA  | ARG | A | 229 | 22.204 | -5.651  | 30.527 | 1.00 | 21.03 |
| ATOM | 1725 | CB  | ARG | A | 229 | 22.833 | -4.291  | 30.221 | 1.00 | 17.71 |
| ATOM | 1726 | CG  | ARG | A | 229 | 23.465 | -4.129  | 28.873 | 1.00 | 18.28 |
| ATOM | 1727 | CD  | ARG | A | 229 | 22.589 | -3.886  | 27.687 | 1.00 | 26.78 |
| ATOM | 1728 | NE  | ARG | A | 229 | 21.245 | -3.355  | 27.849 | 1.00 | 22.41 |
| ATOM | 1729 | CZ  | ARG | A | 229 | 20.263 | -3.671  | 27.008 | 1.00 | 26.65 |
| ATOM | 1730 | NH1 | ARG | A | 229 | 20.514 | -4.494  | 25.992 | 1.00 | 28.43 |
| ATOM | 1731 | NH2 | ARG | A | 229 | 19.031 | -3.197  | 27.144 | 1.00 | 22.64 |
| ATOM | 1732 | C   | ARG | A | 229 | 23.052 | -6.833  | 30.076 | 1.00 | 26.78 |
| ATOM | 1733 | O   | ARG | A | 229 | 22.914 | -7.389  | 28.974 | 1.00 | 22.93 |
| ATOM | 1734 | N   | ASP | A | 230 | 23.970 | -7.282  | 30.931 | 1.00 | 22.22 |
| ATOM | 1735 | CA  | ASP | A | 230 | 24.761 | -8.474  | 30.615 | 1.00 | 19.37 |
| ATOM | 1736 | CB  | ASP | A | 230 | 25.720 | -8.746  | 31.770 | 1.00 | 26.22 |
| ATOM | 1737 | CG  | ASP | A | 230 | 26.764 | -9.808  | 31.496 | 1.00 | 37.14 |
| ATOM | 1738 | OD1 | ASP | A | 230 | 27.772 | -9.830  | 32.234 | 1.00 | 43.30 |
| ATOM | 1739 | OD2 | ASP | A | 230 | 26.579 | -10.609 | 30.558 | 1.00 | 48.34 |
| ATOM | 1740 | C   | ASP | A | 230 | 23.856 | -9.667  | 30.369 | 1.00 | 24.85 |
| ATOM | 1741 | O   | ASP | A | 230 | 24.007 | -10.389 | 29.383 | 1.00 | 27.24 |
| ATOM | 1742 | N   | TYR | A | 231 | 22.897 | -9.868  | 31.276 | 1.00 | 24.39 |
| ATOM | 1743 | CA  | TYR | A | 231 | 21.924 | -10.943 | 31.156 | 1.00 | 17.89 |
| ATOM | 1744 | CB  | TYR | A | 231 | 21.011 | -10.999 | 32.384 | 1.00 | 18.72 |
| ATOM | 1745 | CG  | TYR | A | 231 | 21.604 | -11.752 | 33.540 | 1.00 | 21.03 |
| ATOM | 1746 | CD1 | TYR | A | 231 | 22.218 | -11.040 | 34.559 | 1.00 | 27.60 |
| ATOM | 1747 | CE1 | TYR | A | 231 | 22.770 | -11.713 | 35.627 | 1.00 | 32.43 |
| ATOM | 1748 | CZ  | TYR | A | 231 | 22.716 | -13.085 | 35.692 | 1.00 | 25.45 |
| ATOM | 1749 | OH  | TYR | A | 231 | 23.283 | -13.694 | 36.789 | 1.00 | 36.71 |
| ATOM | 1750 | CE2 | TYR | A | 231 | 22.116 | -13.815 | 34.698 | 1.00 | 23.54 |
| ATOM | 1751 | CD2 | TYR | A | 231 | 21.561 | -13.136 | 33.622 | 1.00 | 30.94 |
| ATOM | 1752 | C   | TYR | A | 231 | 21.006 | -10.771 | 29.954 | 1.00 | 21.66 |
| ATOM | 1753 | O   | TYR | A | 231 | 20.659 | -11.726 | 29.269 | 1.00 | 23.21 |
| ATOM | 1754 | N   | ILE | A | 232 | 20.581 | -9.527  | 29.718 | 1.00 | 16.63 |
| ATOM | 1755 | CA  | ILE | A | 232 | 19.785 | -9.280  | 28.517 | 1.00 | 19.85 |
| ATOM | 1756 | CB  | ILE | A | 232 | 19.349 | -7.808  | 28.395 | 1.00 | 18.50 |
| ATOM | 1757 | CG1 | ILE | A | 232 | 18.391 | -7.370  | 29.499 | 1.00 | 22.29 |
| ATOM | 1758 | CD1 | ILE | A | 232 | 18.084 | -5.901  | 29.616 | 1.00 | 17.14 |
| ATOM | 1759 | CG2 | ILE | A | 232 | 18.773 | -7.570  | 26.999 | 1.00 | 22.60 |
| ATOM | 1760 | C   | ILE | A | 232 | 20.574 | -9.652  | 27.262 | 1.00 | 21.88 |
| ATOM | 1761 | O   | ILE | A | 232 | 20.066 | -10.308 | 26.358 | 1.00 | 24.41 |
| ATOM | 1762 | N   | ASN | A | 233 | 21.840 | -9.242  | 27.197 | 1.00 | 23.34 |
| ATOM | 1763 | CA  | ASN | A | 233 | 22.592 | -9.555  | 25.975 | 1.00 | 30.61 |
| ATOM | 1764 | CB  | ASN | A | 233 | 23.963 | -8.883  | 25.996 | 1.00 | 27.03 |
| ATOM | 1765 | CG  | ASN | A | 233 | 23.869 | -7.379  | 25.800 | 1.00 | 29.17 |
| ATOM | 1766 | OD1 | ASN | A | 233 | 22.902 | -6.849  | 25.248 | 1.00 | 36.95 |
| ATOM | 1767 | ND2 | ASN | A | 233 | 24.882 | -6.648  | 26.251 | 1.00 | 36.00 |

FIGURE 136

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |         |        |      |       |
|------|------|-----|-----|---|-----|--------|---------|--------|------|-------|
| ATOM | 1768 | C   | ASN | A | 233 | 22.705 | -11.062 | 25.808 | 1.00 | 31.90 |
| ATOM | 1769 | O   | ASN | A | 233 | 22.823 | -11.595 | 24.711 | 1.00 | 37.58 |
| ATOM | 1770 | N   | ARG | A | 234 | 22.659 | -11.778 | 26.927 | 1.00 | 29.26 |
| ATOM | 1771 | CA  | ARG | A | 234 | 22.766 | -13.225 | 26.874 | 1.00 | 31.78 |
| ATOM | 1772 | CB  | ARG | A | 234 | 23.465 | -13.746 | 28.129 | 1.00 | 38.80 |
| ATOM | 1773 | CG  | ARG | A | 234 | 24.878 | -13.216 | 28.320 | 1.00 | 43.23 |
| ATOM | 1774 | CD  | ARG | A | 234 | 25.391 | -13.632 | 29.692 | 1.00 | 51.48 |
| ATOM | 1775 | NE  | ARG | A | 234 | 26.840 | -13.511 | 29.800 | 1.00 | 58.62 |
| ATOM | 1776 | CZ  | ARG | A | 234 | 27.670 | -14.516 | 30.055 | 1.00 | 57.56 |
| ATOM | 1777 | NH1 | ARG | A | 234 | 27.201 | -15.746 | 30.232 | 1.00 | 60.00 |
| ATOM | 1778 | NH2 | ARG | A | 234 | 28.975 | -14.277 | 30.128 | 1.00 | 30.80 |
| ATOM | 1779 | C   | ARG | A | 234 | 21.407 | -13.890 | 26.747 | 1.00 | 34.88 |
| ATOM | 1780 | O   | ARG | A | 234 | 21.304 | -15.085 | 27.031 | 1.00 | 32.66 |
| ATOM | 1781 | N   | SER | A | 235 | 20.351 | -13.186 | 26.337 | 1.00 | 24.05 |
| ATOM | 1782 | CA  | SER | A | 235 | 19.065 | -13.884 | 26.273 | 1.00 | 27.03 |
| ATOM | 1783 | CB  | SER | A | 235 | 17.992 | -13.249 | 27.156 | 1.00 | 26.67 |
| ATOM | 1784 | OG  | SER | A | 235 | 18.396 | -13.237 | 28.520 | 1.00 | 34.69 |
| ATOM | 1785 | C   | SER | A | 235 | 18.578 | -13.933 | 24.827 | 1.00 | 31.92 |
| ATOM | 1786 | O   | SER | A | 235 | 17.770 | -13.103 | 24.425 | 1.00 | 28.81 |
| ATOM | 1787 | N   | PRO | A | 236 | 19.099 | -14.914 | 24.105 | 1.00 | 37.48 |
| ATOM | 1788 | CA  | PRO | A | 236 | 18.765 | -15.087 | 22.693 | 1.00 | 39.12 |
| ATOM | 1789 | CB  | PRO | A | 236 | 19.584 | -16.312 | 22.269 | 1.00 | 46.32 |
| ATOM | 1790 | CG  | PRO | A | 236 | 19.866 | -17.038 | 23.546 | 1.00 | 44.02 |
| ATOM | 1791 | CD  | PRO | A | 236 | 20.033 | -15.957 | 24.580 | 1.00 | 42.48 |
| ATOM | 1792 | C   | PRO | A | 236 | 17.279 | -15.378 | 22.517 | 1.00 | 34.00 |
| ATOM | 1793 | O   | PRO | A | 236 | 16.696 | -16.221 | 23.207 | 1.00 | 43.89 |
| ATOM | 1794 | N   | GLY | A | 237 | 16.668 | -14.660 | 21.577 | 1.00 | 27.25 |
| ATOM | 1795 | CA  | GLY | A | 237 | 15.280 | -14.912 | 21.249 | 1.00 | 25.75 |
| ATOM | 1796 | C   | GLY | A | 237 | 14.296 | -14.183 | 22.132 | 1.00 | 21.94 |
| ATOM | 1797 | O   | GLY | A | 237 | 13.109 | -14.257 | 21.848 | 1.00 | 21.04 |
| ATOM | 1798 | N   | ALA | A | 238 | 14.739 | -13.494 | 23.181 | 1.00 | 22.86 |
| ATOM | 1799 | CA  | ALA | A | 238 | 13.836 | -12.838 | 24.112 | 1.00 | 20.89 |
| ATOM | 1800 | CB  | ALA | A | 238 | 14.669 | -12.130 | 25.194 | 1.00 | 22.60 |
| ATOM | 1801 | C   | ALA | A | 238 | 12.923 | -11.807 | 23.470 | 1.00 | 20.68 |
| ATOM | 1802 | O   | ALA | A | 238 | 13.361 | -11.132 | 22.539 | 1.00 | 27.83 |
| ATOM | 1803 | N   | GLY | A | 239 | 11.712 | -11.670 | 23.986 | 1.00 | 18.60 |
| ATOM | 1804 | CA  | GLY | A | 239 | 10.829 | -10.549 | 23.700 | 1.00 | 18.19 |
| ATOM | 1805 | C   | GLY | A | 239 | 11.346 | -9.351  | 24.497 | 1.00 | 15.46 |
| ATOM | 1806 | O   | GLY | A | 239 | 12.521 | -9.353  | 24.887 | 1.00 | 18.43 |
| ATOM | 1807 | N   | PRO | A | 240 | 10.484 | -8.378  | 24.743 | 1.00 | 17.13 |
| ATOM | 1808 | CA  | PRO | A | 240 | 10.889 | -7.184  | 25.496 | 1.00 | 15.73 |
| ATOM | 1809 | CB  | PRO | A | 240 | 9.626  | -6.323  | 25.550 | 1.00 | 18.54 |
| ATOM | 1810 | CG  | PRO | A | 240 | 8.740  | -6.868  | 24.479 | 1.00 | 25.69 |
| ATOM | 1811 | CD  | PRO | A | 240 | 9.073  | -8.329  | 24.350 | 1.00 | 13.87 |
| ATOM | 1812 | C   | PRO | A | 240 | 11.306 | -7.518  | 26.923 | 1.00 | 14.71 |
| ATOM | 1813 | O   | PRO | A | 240 | 10.867 | -8.502  | 27.508 | 1.00 | 14.52 |
| ATOM | 1814 | N   | THR | A | 241 | 12.179 | -6.683  | 27.461 | 1.00 | 13.92 |
| ATOM | 1815 | CA  | THR | A | 241 | 12.533 | -6.674  | 28.869 | 1.00 | 14.60 |
| ATOM | 1816 | CB  | THR | A | 241 | 13.890 | -5.989  | 29.061 | 1.00 | 14.17 |
| ATOM | 1817 | OG1 | THR | A | 241 | 14.893 | -6.769  | 28.389 | 1.00 | 18.17 |
| ATOM | 1818 | CG2 | THR | A | 241 | 14.291 | -5.941  | 30.536 | 1.00 | 17.28 |
| ATOM | 1819 | C   | THR | A | 241 | 11.441 | -5.931  | 29.639 | 1.00 | 16.58 |

**FIGURE 137**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1820 | O   | THR | A | 241 | 11.124 | -4.784 | 29.305 | 1.00 | 13.03 |
| ATOM | 1821 | N   | VAL | A | 242 | 10.856 | -6.571 | 30.646 | 1.00 | 12.88 |
| ATOM | 1822 | CA  | VAL | A | 242 | 9.842  | -5.913 | 31.464 | 1.00 | 9.81  |
| ATOM | 1823 | CB  | VAL | A | 242 | 8.866  | -6.900 | 32.116 | 1.00 | 14.04 |
| ATOM | 1824 | CG1 | VAL | A | 242 | 8.019  | -6.223 | 33.179 | 1.00 | 16.00 |
| ATOM | 1825 | CG2 | VAL | A | 242 | 7.942  | -7.536 | 31.081 | 1.00 | 15.42 |
| ATOM | 1826 | C   | VAL | A | 242 | 10.564 | -5.128 | 32.554 | 1.00 | 12.01 |
| ATOM | 1827 | O   | VAL | A | 242 | 11.501 | -5.623 | 33.171 | 1.00 | 15.03 |
| ATOM | 1828 | N   | VAL | A | 243 | 10.107 | -3.893 | 32.785 | 1.00 | 11.17 |
| ATOM | 1829 | CA  | VAL | A | 243 | 10.668 | -3.065 | 33.838 | 1.00 | 9.13  |
| ATOM | 1830 | CB  | VAL | A | 243 | 11.575 | -1.931 | 33.352 | 1.00 | 15.38 |
| ATOM | 1831 | CG1 | VAL | A | 243 | 12.196 | -1.213 | 34.555 | 1.00 | 10.88 |
| ATOM | 1832 | CG2 | VAL | A | 243 | 12.666 | -2.463 | 32.442 | 1.00 | 12.02 |
| ATOM | 1833 | C   | VAL | A | 243 | 9.482  | -2.452 | 34.574 | 1.00 | 12.00 |
| ATOM | 1834 | O   | VAL | A | 243 | 8.576  | -1.930 | 33.932 | 1.00 | 9.88  |
| ATOM | 1835 | N   | HIS | A | 244 | 9.484  | -2.539 | 35.899 | 1.00 | 11.09 |
| ATOM | 1836 | CA  | HIS | A | 244 | 8.412  | -1.896 | 36.618 | 1.00 | 8.29  |
| ATOM | 1837 | CB  | HIS | A | 244 | 7.205  | -2.846 | 36.762 | 1.00 | 7.72  |
| ATOM | 1838 | CG  | HIS | A | 244 | 7.327  | -3.897 | 37.824 | 1.00 | 15.86 |
| ATOM | 1839 | ND1 | HIS | A | 244 | 7.058  | -3.666 | 39.160 | 1.00 | 14.99 |
| ATOM | 1840 | CE1 | HIS | A | 244 | 7.236  | -4.775 | 39.871 | 1.00 | 13.71 |
| ATOM | 1841 | NE2 | HIS | A | 244 | 7.617  | -5.753 | 39.039 | 1.00 | 16.24 |
| ATOM | 1842 | CD2 | HIS | A | 244 | 7.666  | -5.215 | 37.766 | 1.00 | 15.19 |
| ATOM | 1843 | C   | HIS | A | 244 | 8.890  | -1.434 | 37.999 | 1.00 | 11.45 |
| ATOM | 1844 | O   | HIS | A | 244 | 9.917  | -1.896 | 38.509 | 1.00 | 12.61 |
| ATOM | 1845 | N   | CYS | A | 245 | 8.085  | -0.528 | 38.539 | 1.00 | 18.46 |
| ATOM | 1846 | CA  | CYS | A | 245 | 8.250  | -0.016 | 39.911 | 1.00 | 14.56 |
| ATOM | 1847 | CB  | CYS | A | 245 | 9.019  | 1.304  | 39.865 | 1.00 | 10.22 |
| ATOM | 1848 | SG  | CYS | A | 245 | 8.326  | 2.556  | 38.746 | 1.00 | 14.87 |
| ATOM | 1849 | C   | CYS | A | 245 | 6.876  | 0.022  | 40.549 | 1.00 | 15.86 |
| ATOM | 1850 | O   | CYS | A | 245 | 6.192  | -1.015 | 40.537 | 1.00 | 13.86 |
| ATOM | 1851 | N   | SER | A | 246 | 6.376  | 1.128  | 41.113 | 1.00 | 9.56  |
| ATOM | 1852 | CA  | SER | A | 246 | 4.987  | 1.073  | 41.577 | 1.00 | 9.76  |
| ATOM | 1853 | CB  | SER | A | 246 | 4.844  | 1.783  | 42.926 | 1.00 | 7.75  |
| ATOM | 1854 | OG  | SER | A | 246 | 3.495  | 1.651  | 43.398 | 1.00 | 9.89  |
| ATOM | 1855 | C   | SER | A | 246 | 4.052  | 1.626  | 40.505 | 1.00 | 9.69  |
| ATOM | 1856 | O   | SER | A | 246 | 3.099  | 0.947  | 40.088 | 1.00 | 10.94 |
| ATOM | 1857 | N   | ALA | A | 247 | 4.265  | 2.853  | 40.014 | 1.00 | 15.37 |
| ATOM | 1858 | CA  | ALA | A | 247 | 3.443  | 3.430  | 38.976 | 1.00 | 12.59 |
| ATOM | 1859 | CB  | ALA | A | 247 | 3.411  | 4.964  | 38.966 | 1.00 | 11.87 |
| ATOM | 1860 | C   | ALA | A | 247 | 3.960  | 3.046  | 37.583 | 1.00 | 10.49 |
| ATOM | 1861 | O   | ALA | A | 247 | 3.242  | 3.172  | 36.600 | 1.00 | 15.72 |
| ATOM | 1862 | N   | GLY | A | 248 | 5.216  | 2.627  | 37.542 | 1.00 | 9.25  |
| ATOM | 1863 | CA  | GLY | A | 248 | 5.870  | 2.318  | 36.284 | 1.00 | 13.53 |
| ATOM | 1864 | C   | GLY | A | 248 | 6.210  | 3.615  | 35.570 | 1.00 | 20.73 |
| ATOM | 1865 | O   | GLY | A | 248 | 6.104  | 3.656  | 34.349 | 1.00 | 15.35 |
| ATOM | 1866 | N   | VAL | A | 249 | 6.616  | 4.653  | 36.301 | 1.00 | 14.47 |
| ATOM | 1867 | CA  | VAL | A | 249 | 7.031  | 5.853  | 35.561 | 1.00 | 23.41 |
| ATOM | 1868 | CB  | VAL | A | 249 | 5.942  | 6.948  | 35.534 | 1.00 | 27.80 |
| ATOM | 1869 | CG1 | VAL | A | 249 | 4.675  | 6.441  | 34.850 | 1.00 | 10.99 |
| ATOM | 1870 | CG2 | VAL | A | 249 | 5.615  | 7.470  | 36.930 | 1.00 | 21.36 |
| ATOM | 1871 | C   | VAL | A | 249 | 8.342  | 6.437  | 36.071 | 1.00 | 18.78 |

**FIGURE 138**

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|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1872 | O   | VAL | A | 249 | 9.252  | 6.752  | 35.288 | 1.00 | 16.76 |
| ATOM | 1873 | N   | GLY | A | 250 | 8.505  | 6.625  | 37.372 | 1.00 | 17.57 |
| ATOM | 1874 | CA  | GLY | A | 250 | 9.695  | 7.363  | 37.801 | 1.00 | 15.55 |
| ATOM | 1875 | C   | GLY | A | 250 | 10.939 | 6.526  | 37.860 | 1.00 | 11.84 |
| ATOM | 1876 | O   | GLY | A | 250 | 11.945 | 6.720  | 37.165 | 1.00 | 17.28 |
| ATOM | 1877 | N   | ARG | A | 251 | 10.945 | 5.519  | 38.740 | 1.00 | 11.43 |
| ATOM | 1878 | CA  | ARG | A | 251 | 12.141 | 4.687  | 38.866 | 1.00 | 10.27 |
| ATOM | 1879 | CB  | ARG | A | 251 | 12.050 | 3.844  | 40.148 | 1.00 | 14.41 |
| ATOM | 1880 | CG  | ARG | A | 251 | 12.082 | 4.786  | 41.366 | 1.00 | 15.59 |
| ATOM | 1881 | CD  | ARG | A | 251 | 11.706 | 4.068  | 42.647 | 1.00 | 10.84 |
| ATOM | 1882 | NE  | ARG | A | 251 | 10.278 | 3.795  | 42.721 | 1.00 | 15.91 |
| ATOM | 1883 | CZ  | ARG | A | 251 | 9.729  | 3.085  | 43.709 | 1.00 | 22.05 |
| ATOM | 1884 | NH1 | ARG | A | 251 | 10.528 | 2.610  | 44.665 | 1.00 | 12.86 |
| ATOM | 1885 | NH2 | ARG | A | 251 | 8.413  | 2.887  | 43.697 | 1.00 | 19.96 |
| ATOM | 1886 | C   | ARG | A | 251 | 12.319 | 3.826  | 37.620 | 1.00 | 7.84  |
| ATOM | 1887 | O   | ARG | A | 251 | 13.444 | 3.643  | 37.141 | 1.00 | 13.49 |
| ATOM | 1888 | N   | THR | A | 252 | 11.189 | 3.332  | 37.112 | 1.00 | 10.86 |
| ATOM | 1889 | CA  | THR | A | 252 | 11.278 | 2.605  | 35.826 | 1.00 | 8.96  |
| ATOM | 1890 | CB  | THR | A | 252 | 9.877  | 2.125  | 35.429 | 1.00 | 16.98 |
| ATOM | 1891 | OG1 | THR | A | 252 | 9.509  | 1.052  | 36.311 | 1.00 | 15.33 |
| ATOM | 1892 | CG2 | THR | A | 252 | 9.847  | 1.560  | 34.015 | 1.00 | 18.22 |
| ATOM | 1893 | C   | THR | A | 252 | 11.901 | 3.464  | 34.745 | 1.00 | 13.54 |
| ATOM | 1894 | O   | THR | A | 252 | 12.828 | 3.103  | 34.003 | 1.00 | 14.11 |
| ATOM | 1895 | N   | GLY | A | 253 | 11.410 | 4.690  | 34.594 | 1.00 | 14.04 |
| ATOM | 1896 | CA  | GLY | A | 253 | 11.976 | 5.531  | 33.532 | 1.00 | 16.89 |
| ATOM | 1897 | C   | GLY | A | 253 | 13.426 | 5.881  | 33.711 | 1.00 | 11.18 |
| ATOM | 1898 | O   | GLY | A | 253 | 14.233 | 5.937  | 32.777 | 1.00 | 14.06 |
| ATOM | 1899 | N   | THR | A | 254 | 13.831 | 6.138  | 34.965 | 1.00 | 12.53 |
| ATOM | 1900 | CA  | THR | A | 254 | 15.235 | 6.408  | 35.233 | 1.00 | 13.37 |
| ATOM | 1901 | CB  | THR | A | 254 | 15.455 | 6.837  | 36.695 | 1.00 | 16.96 |
| ATOM | 1902 | OG1 | THR | A | 254 | 14.606 | 7.960  | 36.960 | 1.00 | 17.14 |
| ATOM | 1903 | CG2 | THR | A | 254 | 16.884 | 7.294  | 36.923 | 1.00 | 17.26 |
| ATOM | 1904 | C   | THR | A | 254 | 16.108 | 5.200  | 34.937 | 1.00 | 18.94 |
| ATOM | 1905 | O   | THR | A | 254 | 17.217 | 5.344  | 34.409 | 1.00 | 17.66 |
| ATOM | 1906 | N   | PHE | A | 255 | 15.602 | 4.014  | 35.263 | 1.00 | 11.19 |
| ATOM | 1907 | CA  | PHE | A | 255 | 16.362 | 2.796  | 34.987 | 1.00 | 10.10 |
| ATOM | 1908 | CB  | PHE | A | 255 | 15.617 | 1.534  | 35.479 | 1.00 | 12.68 |
| ATOM | 1909 | CG  | PHE | A | 255 | 16.273 | 0.217  | 35.051 | 1.00 | 13.42 |
| ATOM | 1910 | CD1 | PHE | A | 255 | 17.258 | -0.329 | 35.873 | 1.00 | 14.10 |
| ATOM | 1911 | CE1 | PHE | A | 255 | 17.901 | -1.509 | 35.535 | 1.00 | 15.64 |
| ATOM | 1912 | CZ  | PHE | A | 255 | 17.592 | -2.156 | 34.345 | 1.00 | 14.48 |
| ATOM | 1913 | CE2 | PHE | A | 255 | 16.600 | -1.645 | 33.523 | 1.00 | 15.99 |
| ATOM | 1914 | CD2 | PHE | A | 255 | 15.937 | -0.487 | 33.898 | 1.00 | 19.84 |
| ATOM | 1915 | C   | PHE | A | 255 | 16.626 | 2.687  | 33.493 | 1.00 | 11.10 |
| ATOM | 1916 | O   | PHE | A | 255 | 17.732 | 2.397  | 33.060 | 1.00 | 14.84 |
| ATOM | 1917 | N   | ILE | A | 256 | 15.561 | 2.863  | 32.704 | 1.00 | 14.82 |
| ATOM | 1918 | CA  | ILE | A | 256 | 15.726 | 2.641  | 31.264 | 1.00 | 10.00 |
| ATOM | 1919 | CB  | ILE | A | 256 | 14.352 | 2.607  | 30.589 | 1.00 | 12.80 |
| ATOM | 1920 | CG1 | ILE | A | 256 | 13.558 | 1.345  | 30.943 | 1.00 | 11.66 |
| ATOM | 1921 | CD1 | ILE | A | 256 | 12.084 | 1.457  | 30.602 | 1.00 | 12.54 |
| ATOM | 1922 | CG2 | ILE | A | 256 | 14.463 | 2.826  | 29.091 | 1.00 | 14.64 |
| ATOM | 1923 | C   | ILE | A | 256 | 16.584 | 3.736  | 30.662 | 1.00 | 14.37 |

**FIGURE 139**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1924 | O   | ILE | A | 256 | 17.387 | 3.496  | 29.766 | 1.00 | 20.73 |
| ATOM | 1925 | N   | ALA | A | 257 | 16.399 | 4.970  | 31.154 | 1.00 | 16.70 |
| ATOM | 1926 | CA  | ALA | A | 257 | 17.236 | 6.040  | 30.612 | 1.00 | 12.87 |
| ATOM | 1927 | CB  | ALA | A | 257 | 16.865 | 7.389  | 31.209 | 1.00 | 18.47 |
| ATOM | 1928 | C   | ALA | A | 257 | 18.699 | 5.703  | 30.858 | 1.00 | 19.90 |
| ATOM | 1929 | O   | ALA | A | 257 | 19.567 | 5.851  | 29.993 | 1.00 | 19.76 |
| ATOM | 1930 | N   | LEU | A | 258 | 18.967 | 5.203  | 32.071 | 1.00 | 15.65 |
| ATOM | 1931 | CA  | LEU | A | 258 | 20.358 | 4.894  | 32.395 | 1.00 | 16.29 |
| ATOM | 1932 | CB  | LEU | A | 258 | 20.501 | 4.631  | 33.901 | 1.00 | 18.82 |
| ATOM | 1933 | CG  | LEU | A | 258 | 21.938 | 4.343  | 34.350 | 1.00 | 18.09 |
| ATOM | 1934 | CD1 | LEU | A | 258 | 22.864 | 5.426  | 33.809 | 1.00 | 16.26 |
| ATOM | 1935 | CD2 | LEU | A | 258 | 22.000 | 4.251  | 35.864 | 1.00 | 19.56 |
| ATOM | 1936 | C   | LEU | A | 258 | 20.840 | 3.708  | 31.580 | 1.00 | 21.01 |
| ATOM | 1937 | O   | LEU | A | 258 | 21.974 | 3.651  | 31.110 | 1.00 | 23.61 |
| ATOM | 1938 | N   | ASP | A | 259 | 19.972 | 2.715  | 31.377 | 1.00 | 14.03 |
| ATOM | 1939 | CA  | ASP | A | 259 | 20.372 | 1.573  | 30.549 | 1.00 | 19.00 |
| ATOM | 1940 | CB  | ASP | A | 259 | 19.247 | 0.544  | 30.512 | 1.00 | 16.27 |
| ATOM | 1941 | CG  | ASP | A | 259 | 19.491 | -0.692 | 29.670 | 1.00 | 16.85 |
| ATOM | 1942 | OD1 | ASP | A | 259 | 20.621 | -1.227 | 29.689 | 1.00 | 22.41 |
| ATOM | 1943 | OD2 | ASP | A | 259 | 18.564 | -1.164 | 28.976 | 1.00 | 22.35 |
| ATOM | 1944 | C   | ASP | A | 259 | 20.732 | 2.051  | 29.142 | 1.00 | 24.46 |
| ATOM | 1945 | O   | ASP | A | 259 | 21.715 | 1.611  | 28.532 | 1.00 | 22.50 |
| ATOM | 1946 | N   | ARG | A | 260 | 19.915 | 2.967  | 28.624 | 1.00 | 18.68 |
| ATOM | 1947 | CA  | ARG | A | 260 | 20.166 | 3.492  | 27.277 | 1.00 | 21.73 |
| ATOM | 1948 | CB  | ARG | A | 260 | 18.965 | 4.302  | 26.759 | 1.00 | 19.52 |
| ATOM | 1949 | CG  | ARG | A | 260 | 17.772 | 3.420  | 26.379 | 1.00 | 21.69 |
| ATOM | 1950 | CD  | ARG | A | 260 | 16.687 | 4.238  | 25.678 | 1.00 | 27.46 |
| ATOM | 1951 | NE  | ARG | A | 260 | 17.207 | 4.867  | 24.479 | 1.00 | 35.48 |
| ATOM | 1952 | CZ  | ARG | A | 260 | 16.651 | 5.618  | 23.551 | 1.00 | 36.55 |
| ATOM | 1953 | NH1 | ARG | A | 260 | 15.372 | 5.944  | 23.580 | 1.00 | 47.22 |
| ATOM | 1954 | NH2 | ARG | A | 260 | 17.404 | 6.063  | 22.548 | 1.00 | 36.27 |
| ATOM | 1955 | C   | ARG | A | 260 | 21.432 | 4.331  | 27.217 | 1.00 | 26.15 |
| ATOM | 1956 | O   | ARG | A | 260 | 22.192 | 4.165  | 26.256 | 1.00 | 23.92 |
| ATOM | 1957 | N   | ILE | A | 261 | 21.688 | 5.215  | 28.182 | 1.00 | 26.20 |
| ATOM | 1958 | CA  | ILE | A | 261 | 22.842 | 6.103  | 28.059 | 1.00 | 22.09 |
| ATOM | 1959 | CB  | ILE | A | 261 | 22.764 | 7.376  | 28.922 | 1.00 | 23.64 |
| ATOM | 1960 | CG1 | ILE | A | 261 | 23.001 | 7.148  | 30.418 | 1.00 | 30.05 |
| ATOM | 1961 | CD1 | ILE | A | 261 | 22.191 | 8.055  | 31.328 | 1.00 | 30.61 |
| ATOM | 1962 | CG2 | ILE | A | 261 | 21.452 | 8.105  | 28.674 | 1.00 | 18.34 |
| ATOM | 1963 | C   | ILE | A | 261 | 24.146 | 5.381  | 28.394 | 1.00 | 28.75 |
| ATOM | 1964 | O   | ILE | A | 261 | 25.206 | 5.722  | 27.854 | 1.00 | 36.26 |
| ATOM | 1965 | N   | LEU | A | 262 | 24.110 | 4.384  | 29.276 | 1.00 | 25.96 |
| ATOM | 1966 | CA  | LEU | A | 262 | 25.364 | 3.663  | 29.544 | 1.00 | 24.13 |
| ATOM | 1967 | CB  | LEU | A | 262 | 25.207 | 2.686  | 30.699 | 1.00 | 24.26 |
| ATOM | 1968 | CG  | LEU | A | 262 | 25.112 | 3.236  | 32.123 | 1.00 | 20.71 |
| ATOM | 1969 | CD1 | LEU | A | 262 | 25.079 | 2.071  | 33.101 | 1.00 | 24.55 |
| ATOM | 1970 | CD2 | LEU | A | 262 | 26.257 | 4.176  | 32.453 | 1.00 | 23.31 |
| ATOM | 1971 | C   | LEU | A | 262 | 25.812 | 2.958  | 28.271 | 1.00 | 29.49 |
| ATOM | 1972 | O   | LEU | A | 262 | 27.004 | 2.863  | 27.968 | 1.00 | 38.42 |
| ATOM | 1973 | N   | GLN | A | 263 | 24.851 | 2.454  | 27.494 | 1.00 | 29.52 |
| ATOM | 1974 | CA  | GLN | A | 263 | 25.225 | 1.863  | 26.204 | 1.00 | 35.18 |
| ATOM | 1975 | CB  | GLN | A | 263 | 24.015 | 1.216  | 25.545 | 1.00 | 34.97 |

**FIGURE 140**



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1976 | CG  | GLN | A | 263 | 23.632 | -0.140 | 26.125 | 1.00 | 36.78 |
| ATOM | 1977 | CD  | GLN | A | 263 | 22.277 | -0.630 | 25.661 | 1.00 | 34.45 |
| ATOM | 1978 | OE1 | GLN | A | 263 | 22.167 | -1.327 | 24.653 | 1.00 | 32.02 |
| ATOM | 1979 | NE2 | GLN | A | 263 | 21.219 | -0.276 | 26.388 | 1.00 | 29.68 |
| ATOM | 1980 | C   | GLN | A | 263 | 25.867 | 2.912  | 25.300 | 1.00 | 38.62 |
| ATOM | 1981 | O   | GLN | A | 263 | 26.927 | 2.694  | 24.702 | 1.00 | 44.23 |
| ATOM | 1982 | N   | GLN | A | 264 | 25.255 | 4.084  | 25.187 | 1.00 | 40.04 |
| ATOM | 1983 | CA  | GLN | A | 264 | 25.848 | 5.189  | 24.439 | 1.00 | 37.35 |
| ATOM | 1984 | CB  | GLN | A | 264 | 25.018 | 6.461  | 24.597 | 1.00 | 30.80 |
| ATOM | 1985 | CG  | GLN | A | 264 | 23.739 | 6.499  | 23.777 | 1.00 | 28.49 |
| ATOM | 1986 | CD  | GLN | A | 264 | 22.842 | 7.650  | 24.195 | 1.00 | 36.13 |
| ATOM | 1987 | OE1 | GLN | A | 264 | 23.318 | 8.630  | 24.778 | 1.00 | 35.61 |
| ATOM | 1988 | NE2 | GLN | A | 264 | 21.552 | 7.519  | 23.905 | 1.00 | 30.19 |
| ATOM | 1989 | C   | GLN | A | 264 | 27.280 | 5.460  | 24.900 | 1.00 | 46.87 |
| ATOM | 1990 | O   | GLN | A | 264 | 28.192 | 5.539  | 24.076 | 1.00 | 59.11 |
| ATOM | 1991 | N   | LEU | A | 265 | 27.474 | 5.599  | 26.210 | 1.00 | 44.30 |
| ATOM | 1992 | CA  | LEU | A | 265 | 28.805 | 5.808  | 26.774 | 1.00 | 44.22 |
| ATOM | 1993 | CB  | LEU | A | 265 | 28.794 | 5.779  | 28.295 | 1.00 | 47.83 |
| ATOM | 1994 | CG  | LEU | A | 265 | 28.082 | 6.900  | 29.043 | 1.00 | 50.56 |
| ATOM | 1995 | CD1 | LEU | A | 265 | 28.140 | 6.641  | 30.544 | 1.00 | 39.48 |
| ATOM | 1996 | CD2 | LEU | A | 265 | 28.678 | 8.255  | 28.696 | 1.00 | 54.16 |
| ATOM | 1997 | C   | LEU | A | 265 | 29.763 | 4.736  | 26.265 | 1.00 | 45.05 |
| ATOM | 1998 | O   | LEU | A | 265 | 30.912 | 5.011  | 25.925 | 1.00 | 54.65 |
| ATOM | 1999 | N   | ASP | A | 266 | 29.280 | 3.495  | 26.209 | 1.00 | 40.79 |
| ATOM | 2000 | CA  | ASP | A | 266 | 30.137 | 2.440  | 25.670 | 1.00 | 47.27 |
| ATOM | 2001 | CB  | ASP | A | 266 | 29.739 | 1.083  | 26.257 | 1.00 | 43.47 |
| ATOM | 2002 | CG  | ASP | A | 266 | 30.102 | 0.960  | 27.721 | 1.00 | 44.36 |
| ATOM | 2003 | OD1 | ASP | A | 266 | 31.196 | 1.428  | 28.101 | 1.00 | 58.24 |
| ATOM | 2004 | OD2 | ASP | A | 266 | 29.297 | 0.391  | 28.488 | 1.00 | 53.34 |
| ATOM | 2005 | C   | ASP | A | 266 | 30.066 | 2.396  | 24.154 | 1.00 | 58.50 |
| ATOM | 2006 | O   | ASP | A | 266 | 30.476 | 1.429  | 23.506 | 1.00 | 56.64 |
| ATOM | 2007 | N   | SER | A | 267 | 29.538 | 3.434  | 23.497 | 1.00 | 67.18 |
| ATOM | 2008 | CA  | SER | A | 267 | 29.465 | 3.282  | 22.038 | 1.00 | 73.64 |
| ATOM | 2009 | CB  | SER | A | 267 | 28.110 | 2.671  | 21.667 | 1.00 | 75.02 |
| ATOM | 2010 | OG  | SER | A | 267 | 28.161 | 1.258  | 21.786 | 1.00 | 72.08 |
| ATOM | 2011 | C   | SER | A | 267 | 29.693 | 4.592  | 21.301 | 1.00 | 81.56 |
| ATOM | 2012 | O   | SER | A | 267 | 30.504 | 4.666  | 20.376 | 1.00 | 96.45 |
| ATOM | 2013 | N   | LYS | A | 268 | 28.971 | 5.630  | 21.705 | 1.00 | 82.73 |
| ATOM | 2014 | CA  | LYS | A | 268 | 29.039 | 6.931  | 21.064 | 1.00 | 81.39 |
| ATOM | 2015 | CB  | LYS | A | 268 | 27.736 | 7.709  | 21.286 | 1.00 | 92.60 |
| ATOM | 2016 | CG  | LYS | A | 268 | 26.518 | 7.115  | 20.597 | 1.00 | 98.30 |
| ATOM | 2017 | CD  | LYS | A | 268 | 25.516 | 8.187  | 20.194 | 1.00 | 99.41 |
| ATOM | 2018 | CE  | LYS | A | 268 | 25.288 | 9.191  | 21.312 | 1.00 | 97.43 |
| ATOM | 2019 | NZ  | LYS | A | 268 | 23.896 | 9.151  | 21.836 | 1.00 | 86.39 |
| ATOM | 2020 | C   | LYS | A | 268 | 30.209 | 7.766  | 21.583 | 1.00 | 67.12 |
| ATOM | 2021 | O   | LYS | A | 268 | 30.930 | 7.340  | 22.478 | 1.00 | 61.30 |
| ATOM | 2022 | N   | ASP | A | 269 | 30.340 | 8.941  | 20.995 | 1.00 | 57.55 |
| ATOM | 2023 | CA  | ASP | A | 269 | 31.277 | 9.986  | 21.380 | 1.00 | 61.48 |
| ATOM | 2024 | CB  | ASP | A | 269 | 31.994 | 10.514 | 20.137 | 1.00 | 71.27 |
| ATOM | 2025 | CG  | ASP | A | 269 | 31.482 | 9.789  | 18.899 | 1.00 | 80.60 |
| ATOM | 2026 | OD1 | ASP | A | 269 | 32.270 | 9.060  | 18.261 | 1.00 | 87.05 |
| ATOM | 2027 | OD2 | ASP | A | 269 | 30.283 | 9.954  | 18.585 | 1.00 | 82.09 |

**FIGURE 141**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2028 | C   | ASP | A | 269 | 30.498 | 11.081 | 22.096 | 1.00 | 54.39 |
| ATOM | 2029 | O   | ASP | A | 269 | 30.997 | 12.070 | 22.621 | 1.00 | 37.16 |
| ATOM | 2030 | N   | SER | A | 270 | 29.183 | 10.843 | 22.108 | 1.00 | 44.05 |
| ATOM | 2031 | CA  | SER | A | 270 | 28.290 | 11.754 | 22.805 | 1.00 | 48.15 |
| ATOM | 2032 | CB  | SER | A | 270 | 27.593 | 12.687 | 21.814 | 1.00 | 54.66 |
| ATOM | 2033 | OG  | SER | A | 270 | 27.367 | 12.009 | 20.588 | 1.00 | 61.37 |
| ATOM | 2034 | C   | SER | A | 270 | 27.261 | 10.971 | 23.609 | 1.00 | 44.27 |
| ATOM | 2035 | O   | SER | A | 270 | 27.045 | 9.781  | 23.410 | 1.00 | 33.61 |
| ATOM | 2036 | N   | VAL | A | 271 | 26.613 | 11.652 | 24.544 | 1.00 | 41.56 |
| ATOM | 2037 | CA  | VAL | A | 271 | 25.550 | 10.966 | 25.288 | 1.00 | 44.74 |
| ATOM | 2038 | CB  | VAL | A | 271 | 25.984 | 10.636 | 26.722 | 1.00 | 43.78 |
| ATOM | 2039 | CG1 | VAL | A | 271 | 26.585 | 11.844 | 27.428 | 1.00 | 22.16 |
| ATOM | 2040 | CG2 | VAL | A | 271 | 24.822 | 10.084 | 27.544 | 1.00 | 24.65 |
| ATOM | 2041 | C   | VAL | A | 271 | 24.316 | 11.852 | 25.185 | 1.00 | 43.38 |
| ATOM | 2042 | O   | VAL | A | 271 | 24.418 | 13.084 | 25.177 | 1.00 | 32.23 |
| ATOM | 2043 | N   | ASP | A | 272 | 23.146 | 11.232 | 25.058 | 1.00 | 35.09 |
| ATOM | 2044 | CA  | ASP | A | 272 | 21.929 | 12.022 | 24.874 | 1.00 | 36.34 |
| ATOM | 2045 | CB  | ASP | A | 272 | 21.317 | 11.723 | 23.500 | 1.00 | 28.68 |
| ATOM | 2046 | CG  | ASP | A | 272 | 20.345 | 12.806 | 23.075 | 1.00 | 25.29 |
| ATOM | 2047 | OD1 | ASP | A | 272 | 20.363 | 13.875 | 23.726 | 1.00 | 33.02 |
| ATOM | 2048 | OD2 | ASP | A | 272 | 19.581 | 12.595 | 22.112 | 1.00 | 37.57 |
| ATOM | 2049 | C   | ASP | A | 272 | 20.936 | 11.754 | 25.993 | 1.00 | 33.69 |
| ATOM | 2050 | O   | ASP | A | 272 | 19.969 | 11.023 | 25.818 | 1.00 | 35.34 |
| ATOM | 2051 | N   | ILE | A | 273 | 21.171 | 12.338 | 27.166 | 1.00 | 29.39 |
| ATOM | 2052 | CA  | ILE | A | 273 | 20.262 | 12.106 | 28.281 | 1.00 | 31.17 |
| ATOM | 2053 | CB  | ILE | A | 273 | 20.840 | 12.632 | 29.611 | 1.00 | 33.58 |
| ATOM | 2054 | CG1 | ILE | A | 273 | 22.112 | 11.900 | 30.045 | 1.00 | 34.59 |
| ATOM | 2055 | CD1 | ILE | A | 273 | 22.785 | 12.475 | 31.270 | 1.00 | 32.68 |
| ATOM | 2056 | CG2 | ILE | A | 273 | 19.793 | 12.604 | 30.714 | 1.00 | 21.45 |
| ATOM | 2057 | C   | ILE | A | 273 | 18.909 | 12.754 | 28.018 | 1.00 | 36.45 |
| ATOM | 2058 | O   | ILE | A | 273 | 17.873 | 12.152 | 28.319 | 1.00 | 29.72 |
| ATOM | 2059 | N   | TYR | A | 274 | 18.921 | 13.967 | 27.465 | 1.00 | 23.18 |
| ATOM | 2060 | CA  | TYR | A | 274 | 17.658 | 14.663 | 27.204 | 1.00 | 23.24 |
| ATOM | 2061 | CB  | TYR | A | 274 | 17.927 | 16.065 | 26.659 | 1.00 | 21.30 |
| ATOM | 2062 | CG  | TYR | A | 274 | 16.720 | 16.885 | 26.286 | 1.00 | 28.11 |
| ATOM | 2063 | CD1 | TYR | A | 274 | 16.099 | 17.722 | 27.205 | 1.00 | 30.12 |
| ATOM | 2064 | CE1 | TYR | A | 274 | 14.991 | 18.475 | 26.855 | 1.00 | 36.51 |
| ATOM | 2065 | CZ  | TYR | A | 274 | 14.486 | 18.401 | 25.576 | 1.00 | 39.07 |
| ATOM | 2066 | OH  | TYR | A | 274 | 13.384 | 19.137 | 25.206 | 1.00 | 39.75 |
| ATOM | 2067 | CE2 | TYR | A | 274 | 15.082 | 17.578 | 24.641 | 1.00 | 33.12 |
| ATOM | 2068 | CD2 | TYR | A | 274 | 16.183 | 16.837 | 25.003 | 1.00 | 30.11 |
| ATOM | 2069 | C   | TYR | A | 274 | 16.810 | 13.851 | 26.229 | 1.00 | 23.51 |
| ATOM | 2070 | O   | TYR | A | 274 | 15.604 | 13.715 | 26.425 | 1.00 | 26.03 |
| ATOM | 2071 | N   | GLY | A | 275 | 17.435 | 13.350 | 25.181 | 1.00 | 21.12 |
| ATOM | 2072 | CA  | GLY | A | 275 | 16.774 | 12.633 | 24.100 | 1.00 | 24.69 |
| ATOM | 2073 | C   | GLY | A | 275 | 16.230 | 11.296 | 24.575 | 1.00 | 30.05 |
| ATOM | 2074 | O   | GLY | A | 275 | 15.206 | 10.793 | 24.115 | 1.00 | 26.82 |
| ATOM | 2075 | N   | ALA | A | 276 | 16.950 | 10.705 | 25.531 | 1.00 | 28.67 |
| ATOM | 2076 | CA  | ALA | A | 276 | 16.477 | 9.436  | 26.087 | 1.00 | 28.22 |
| ATOM | 2077 | CB  | ALA | A | 276 | 17.538 | 8.828  | 26.980 | 1.00 | 23.79 |
| ATOM | 2078 | C   | ALA | A | 276 | 15.165 | 9.685  | 26.816 | 1.00 | 25.48 |
| ATOM | 2079 | O   | ALA | A | 276 | 14.174 | 8.993  | 26.612 | 1.00 | 21.68 |

**FIGURE 142**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2080 | N   | VAL | A | 277 | 15.134 | 10.709 | 27.669 | 1.00 | 19.63 |
| ATOM | 2081 | CA  | VAL | A | 277 | 13.928 | 10.960 | 28.450 | 1.00 | 18.94 |
| ATOM | 2082 | CB  | VAL | A | 277 | 14.184 | 11.957 | 29.592 | 1.00 | 18.63 |
| ATOM | 2083 | CG1 | VAL | A | 277 | 12.919 | 12.193 | 30.417 | 1.00 | 19.37 |
| ATOM | 2084 | CG2 | VAL | A | 277 | 15.308 | 11.457 | 30.497 | 1.00 | 23.87 |
| ATOM | 2085 | C   | VAL | A | 277 | 12.820 | 11.458 | 27.538 | 1.00 | 22.49 |
| ATOM | 2086 | O   | VAL | A | 277 | 11.642 | 11.184 | 27.731 | 1.00 | 18.77 |
| ATOM | 2087 | N   | HIS | A | 278 | 13.225 | 12.224 | 26.522 | 1.00 | 20.21 |
| ATOM | 2088 | CA  | HIS | A | 278 | 12.220 | 12.729 | 25.587 | 1.00 | 20.77 |
| ATOM | 2089 | CB  | HIS | A | 278 | 12.888 | 13.637 | 24.538 | 1.00 | 19.46 |
| ATOM | 2090 | CG  | HIS | A | 278 | 11.915 | 14.109 | 23.501 | 1.00 | 27.73 |
| ATOM | 2091 | ND1 | HIS | A | 278 | 11.599 | 13.361 | 22.387 | 1.00 | 25.43 |
| ATOM | 2092 | CE1 | HIS | A | 278 | 10.714 | 14.023 | 21.661 | 1.00 | 26.78 |
| ATOM | 2093 | NE2 | HIS | A | 278 | 10.441 | 15.169 | 22.258 | 1.00 | 30.40 |
| ATOM | 2094 | CD2 | HIS | A | 278 | 11.180 | 15.243 | 23.412 | 1.00 | 29.32 |
| ATOM | 2095 | C   | HIS | A | 278 | 11.505 | 11.529 | 24.958 | 1.00 | 17.28 |
| ATOM | 2096 | O   | HIS | A | 278 | 10.282 | 11.474 | 24.934 | 1.00 | 19.03 |
| ATOM | 2097 | N   | ASP | A | 279 | 12.283 | 10.576 | 24.448 | 1.00 | 19.78 |
| ATOM | 2098 | CA  | ASP | A | 279 | 11.736 | 9.408  | 23.766 | 1.00 | 23.11 |
| ATOM | 2099 | CB  | ASP | A | 279 | 12.830 | 8.508  | 23.192 | 1.00 | 31.32 |
| ATOM | 2100 | CG  | ASP | A | 279 | 12.445 | 7.760  | 21.931 | 1.00 | 41.53 |
| ATOM | 2101 | OD1 | ASP | A | 279 | 11.649 | 8.288  | 21.124 | 1.00 | 44.27 |
| ATOM | 2102 | OD2 | ASP | A | 279 | 12.924 | 6.627  | 21.689 | 1.00 | 31.21 |
| ATOM | 2103 | C   | ASP | A | 279 | 10.860 | 8.613  | 24.733 | 1.00 | 16.22 |
| ATOM | 2104 | O   | ASP | A | 279 | 9.794  | 8.139  | 24.359 | 1.00 | 17.27 |
| ATOM | 2105 | N   | LEU | A | 280 | 11.327 | 8.486  | 25.974 | 1.00 | 18.29 |
| ATOM | 2106 | CA  | LEU | A | 280 | 10.517 | 7.786  | 26.974 | 1.00 | 19.74 |
| ATOM | 2107 | CB  | LEU | A | 280 | 11.270 | 7.751  | 28.301 | 1.00 | 15.55 |
| ATOM | 2108 | CG  | LEU | A | 280 | 12.388 | 6.723  | 28.463 | 1.00 | 26.78 |
| ATOM | 2109 | CD1 | LEU | A | 280 | 13.190 | 6.944  | 29.734 | 1.00 | 23.32 |
| ATOM | 2110 | CD2 | LEU | A | 280 | 11.836 | 5.303  | 28.501 | 1.00 | 32.51 |
| ATOM | 2111 | C   | LEU | A | 280 | 9.162  | 8.456  | 27.109 | 1.00 | 19.74 |
| ATOM | 2112 | O   | LEU | A | 280 | 8.100  | 7.831  | 27.099 | 1.00 | 15.47 |
| ATOM | 2113 | N   | ARG | A | 281 | 9.152  | 9.785  | 27.240 | 1.00 | 17.32 |
| ATOM | 2114 | CA  | ARG | A | 281 | 7.931  | 10.535 | 27.402 | 1.00 | 18.47 |
| ATOM | 2115 | CB  | ARG | A | 281 | 8.195  | 12.047 | 27.522 | 1.00 | 21.28 |
| ATOM | 2116 | CG  | ARG | A | 281 | 9.115  | 12.436 | 28.661 | 1.00 | 29.75 |
| ATOM | 2117 | CD  | ARG | A | 281 | 8.318  | 12.580 | 29.951 | 1.00 | 34.02 |
| ATOM | 2118 | NE  | ARG | A | 281 | 9.199  | 13.015 | 31.026 | 1.00 | 37.36 |
| ATOM | 2119 | CZ  | ARG | A | 281 | 8.851  | 13.737 | 32.071 | 1.00 | 39.23 |
| ATOM | 2120 | NH1 | ARG | A | 281 | 7.595  | 14.129 | 32.206 | 1.00 | 60.17 |
| ATOM | 2121 | NH2 | ARG | A | 281 | 9.769  | 14.055 | 32.972 | 1.00 | 36.32 |
| ATOM | 2122 | C   | ARG | A | 281 | 6.987  | 10.381 | 26.220 | 1.00 | 16.87 |
| ATOM | 2123 | O   | ARG | A | 281 | 5.785  | 10.568 | 26.424 | 1.00 | 18.99 |
| ATOM | 2124 | N   | LEU | A | 282 | 7.549  | 10.111 | 25.034 | 1.00 | 15.85 |
| ATOM | 2125 | CA  | LEU | A | 282 | 6.620  | 9.977  | 23.899 | 1.00 | 17.78 |
| ATOM | 2126 | CB  | LEU | A | 282 | 7.338  | 9.907  | 22.559 | 1.00 | 21.15 |
| ATOM | 2127 | CG  | LEU | A | 282 | 8.060  | 11.126 | 21.997 | 1.00 | 32.88 |
| ATOM | 2128 | CD1 | LEU | A | 282 | 8.732  | 10.767 | 20.673 | 1.00 | 28.74 |
| ATOM | 2129 | CD2 | LEU | A | 282 | 7.133  | 12.311 | 21.783 | 1.00 | 24.88 |
| ATOM | 2130 | C   | LEU | A | 282 | 5.763  | 8.721  | 24.078 | 1.00 | 18.42 |
| ATOM | 2131 | O   | LEU | A | 282 | 4.658  | 8.631  | 23.532 | 1.00 | 21.04 |

**FIGURE 143**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2132 | N   | HIS | A | 283 | 6.263  | 7.739  | 24.823 | 1.00 | 16.75 |
| ATOM | 2133 | CA  | HIS | A | 283 | 5.574  | 6.450  | 24.905 | 1.00 | 17.03 |
| ATOM | 2134 | CB  | HIS | A | 283 | 6.621  | 5.350  | 24.644 | 1.00 | 17.45 |
| ATOM | 2135 | CG  | HIS | A | 283 | 7.133  | 5.464  | 23.234 | 1.00 | 19.75 |
| ATOM | 2136 | ND1 | HIS | A | 283 | 6.502  | 4.868  | 22.169 | 1.00 | 24.70 |
| ATOM | 2137 | CE1 | HIS | A | 283 | 7.156  | 5.149  | 21.056 | 1.00 | 24.61 |
| ATOM | 2138 | NE2 | HIS | A | 283 | 8.191  | 5.913  | 21.353 | 1.00 | 23.33 |
| ATOM | 2139 | CD2 | HIS | A | 283 | 8.186  | 6.126  | 22.714 | 1.00 | 25.41 |
| ATOM | 2140 | C   | HIS | A | 283 | 4.831  | 6.199  | 26.209 | 1.00 | 17.38 |
| ATOM | 2141 | O   | HIS | A | 283 | 3.932  | 5.336  | 26.249 | 1.00 | 12.95 |
| ATOM | 2142 | N   | ARG | A | 284 | 5.125  | 6.923  | 27.282 | 1.00 | 12.46 |
| ATOM | 2143 | CA  | ARG | A | 284 | 4.367  | 6.792  | 28.527 | 1.00 | 12.55 |
| ATOM | 2144 | CB  | ARG | A | 284 | 4.869  | 5.622  | 29.366 | 1.00 | 13.17 |
| ATOM | 2145 | CG  | ARG | A | 284 | 4.072  | 5.322  | 30.633 | 1.00 | 10.87 |
| ATOM | 2146 | CD  | ARG | A | 284 | 4.464  | 3.909  | 31.097 | 1.00 | 17.92 |
| ATOM | 2147 | NE  | ARG | A | 284 | 3.933  | 3.546  | 32.404 | 1.00 | 11.92 |
| ATOM | 2148 | CZ  | ARG | A | 284 | 2.752  | 2.965  | 32.601 | 1.00 | 15.19 |
| ATOM | 2149 | NH1 | ARG | A | 284 | 1.953  | 2.675  | 31.577 | 1.00 | 12.14 |
| ATOM | 2150 | NH2 | ARG | A | 284 | 2.348  | 2.666  | 33.837 | 1.00 | 11.55 |
| ATOM | 2151 | C   | ARG | A | 284 | 4.496  | 8.059  | 29.372 | 1.00 | 12.80 |
| ATOM | 2152 | O   | ARG | A | 284 | 5.555  | 8.665  | 29.370 | 1.00 | 13.52 |
| ATOM | 2153 | N   | VAL | A | 285 | 3.435  | 8.425  | 30.059 | 1.00 | 17.40 |
| ATOM | 2154 | CA  | VAL | A | 285 | 3.419  | 9.665  | 30.847 | 1.00 | 15.70 |
| ATOM | 2155 | CB  | VAL | A | 285 | 1.998  | 9.930  | 31.379 | 1.00 | 18.07 |
| ATOM | 2156 | CG1 | VAL | A | 285 | 1.657  | 8.972  | 32.521 | 1.00 | 14.53 |
| ATOM | 2157 | CG2 | VAL | A | 285 | 1.848  | 11.380 | 31.837 | 1.00 | 21.60 |
| ATOM | 2158 | C   | VAL | A | 285 | 4.429  | 9.640  | 31.982 | 1.00 | 24.82 |
| ATOM | 2159 | O   | VAL | A | 285 | 4.767  | 8.581  | 32.511 | 1.00 | 18.02 |
| ATOM | 2160 | N   | HIS | A | 286 | 4.926  | 10.823 | 32.336 | 1.00 | 22.81 |
| ATOM | 2161 | CA  | HIS | A | 286 | 5.818  | 11.084 | 33.440 | 1.00 | 20.84 |
| ATOM | 2162 | CB  | HIS | A | 286 | 5.069  | 10.872 | 34.768 | 1.00 | 24.11 |
| ATOM | 2163 | CG  | HIS | A | 286 | 3.818  | 11.663 | 34.965 | 1.00 | 28.34 |
| ATOM | 2164 | ND1 | HIS | A | 286 | 3.763  | 13.039 | 34.936 | 1.00 | 28.84 |
| ATOM | 2165 | CE1 | HIS | A | 286 | 2.526  | 13.448 | 35.147 | 1.00 | 28.83 |
| ATOM | 2166 | NE2 | HIS | A | 286 | 1.766  | 12.380 | 35.317 | 1.00 | 32.75 |
| ATOM | 2167 | CD2 | HIS | A | 286 | 2.548  | 11.255 | 35.216 | 1.00 | 26.94 |
| ATOM | 2168 | C   | HIS | A | 286 | 7.084  | 10.232 | 33.510 | 1.00 | 21.64 |
| ATOM | 2169 | O   | HIS | A | 286 | 7.661  | 10.218 | 34.615 | 1.00 | 26.93 |
| ATOM | 2170 | N   | MET | A | 287 | 7.550  | 9.548  | 32.468 | 1.00 | 13.96 |
| ATOM | 2171 | CA  | MET | A | 287 | 8.792  | 8.783  | 32.560 | 1.00 | 13.56 |
| ATOM | 2172 | CB  | MET | A | 287 | 9.223  | 8.171  | 31.264 | 1.00 | 16.67 |
| ATOM | 2173 | CG  | MET | A | 287 | 8.741  | 6.954  | 30.564 | 1.00 | 32.18 |
| ATOM | 2174 | SD  | MET | A | 287 | 8.371  | 5.520  | 31.623 | 1.00 | 31.45 |
| ATOM | 2175 | CE  | MET | A | 287 | 6.873  | 6.119  | 32.287 | 1.00 | 12.41 |
| ATOM | 2176 | C   | MET | A | 287 | 9.919  | 9.708  | 33.070 | 1.00 | 31.47 |
| ATOM | 2177 | O   | MET | A | 287 | 10.136 | 10.813 | 32.556 | 1.00 | 27.35 |
| ATOM | 2178 | N   | VAL | A | 288 | 10.581 | 9.213  | 34.107 | 1.00 | 19.43 |
| ATOM | 2179 | CA  | VAL | A | 288 | 11.539 | 9.968  | 34.906 | 1.00 | 20.51 |
| ATOM | 2180 | CB  | VAL | A | 288 | 12.719 | 10.500 | 34.089 | 1.00 | 18.73 |
| ATOM | 2181 | CG1 | VAL | A | 288 | 13.598 | 11.361 | 34.989 | 1.00 | 27.60 |
| ATOM | 2182 | CG2 | VAL | A | 288 | 13.506 | 9.344  | 33.475 | 1.00 | 16.71 |
| ATOM | 2183 | C   | VAL | A | 288 | 10.780 | 11.107 | 35.584 | 1.00 | 24.09 |

**FIGURE 144**

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 2184 | O   | VAL | A | 288 | 10.586 | 12.174 | 35.013 | 1.00 | 30.01  |
| ATOM | 2185 | N   | GLN | A | 289 | 10.325 | 10.820 | 36.799 | 1.00 | 20.54  |
| ATOM | 2186 | CA  | GLN | A | 289 | 9.237  | 11.559 | 37.407 | 1.00 | 28.07  |
| ATOM | 2187 | CB  | GLN | A | 289 | 8.381  | 10.595 | 38.239 | 1.00 | 31.79  |
| ATOM | 2188 | CG  | GLN | A | 289 | 7.078  | 11.185 | 38.754 | 1.00 | 34.58  |
| ATOM | 2189 | CD  | GLN | A | 289 | 7.101  | 11.363 | 40.266 | 1.00 | 35.98  |
| ATOM | 2190 | OE1 | GLN | A | 289 | 7.791  | 10.623 | 40.972 | 1.00 | 26.51  |
| ATOM | 2191 | NE2 | GLN | A | 289 | 6.346  | 12.347 | 40.753 | 1.00 | 36.09  |
| ATOM | 2192 | C   | GLN | A | 289 | 9.689  | 12.720 | 38.278 | 1.00 | 33.05  |
| ATOM | 2193 | O   | GLN | A | 289 | 8.858  | 13.599 | 38.525 | 1.00 | 35.10  |
| ATOM | 2194 | N   | THR | A | 290 | 10.936 | 12.736 | 38.736 | 1.00 | 30.88  |
| ATOM | 2195 | CA  | THR | A | 290 | 11.372 | 13.920 | 39.491 | 1.00 | 28.02  |
| ATOM | 2196 | CB  | THR | A | 290 | 11.590 | 13.611 | 40.984 | 1.00 | 29.29  |
| ATOM | 2197 | OG1 | THR | A | 290 | 12.661 | 12.677 | 41.160 | 1.00 | 35.40  |
| ATOM | 2198 | CG2 | THR | A | 290 | 10.331 | 12.980 | 41.563 | 1.00 | 24.35  |
| ATOM | 2199 | C   | THR | A | 290 | 12.639 | 14.518 | 38.909 | 1.00 | 23.50  |
| ATOM | 2200 | O   | THR | A | 290 | 13.496 | 13.903 | 38.287 | 1.00 | 21.72  |
| ATOM | 2201 | N   | GLU | A | 291 | 12.806 | 15.830 | 39.108 | 1.00 | 33.06  |
| ATOM | 2202 | CA  | GLU | A | 291 | 13.996 | 16.481 | 38.534 | 1.00 | 26.38  |
| ATOM | 2203 | CB  | GLU | A | 291 | 13.849 | 17.986 | 38.728 | 1.00 | 36.13  |
| ATOM | 2204 | CG  | GLU | A | 291 | 14.794 | 18.656 | 39.697 | 1.00 | 47.55  |
| ATOM | 2205 | CD  | GLU | A | 291 | 15.133 | 20.079 | 39.279 | 1.00 | 50.62  |
| ATOM | 2206 | OE1 | GLU | A | 291 | 16.237 | 20.541 | 39.645 | 1.00 | 58.58  |
| ATOM | 2207 | OE2 | GLU | A | 291 | 14.306 | 20.719 | 38.593 | 1.00 | 33.56  |
| ATOM | 2208 | C   | GLU | A | 291 | 15.255 | 15.901 | 39.151 | 1.00 | 20.43  |
| ATOM | 2209 | O   | GLU | A | 291 | 16.325 | 15.881 | 38.543 | 1.00 | 24.26  |
| ATOM | 2210 | N   | CYS | A | 292 | 15.139 | 15.407 | 40.386 | 1.00 | 20.50  |
| ATOM | 2211 | CA  | CYS | A | 292 | 16.308 | 14.825 | 41.039 | 1.00 | 19.18  |
| ATOM | 2212 | CB  | CYS | A | 292 | 16.040 | 14.535 | 42.517 | 1.00 | 31.41  |
| ATOM | 2213 | SG  | CYS | A | 292 | 17.552 | 14.159 | 43.444 | 1.00 | 101.20 |
| ATOM | 2214 | C   | CYS | A | 292 | 16.721 | 13.542 | 40.335 | 1.00 | 20.87  |
| ATOM | 2215 | O   | CYS | A | 292 | 17.899 | 13.219 | 40.202 | 1.00 | 24.99  |
| ATOM | 2216 | N   | GLN | A | 293 | 15.718 | 12.795 | 39.862 | 1.00 | 26.29  |
| ATOM | 2217 | CA  | GLN | A | 293 | 16.062 | 11.613 | 39.055 | 1.00 | 22.01  |
| ATOM | 2218 | CB  | GLN | A | 293 | 14.785 | 10.827 | 38.720 | 1.00 | 22.44  |
| ATOM | 2219 | CG  | GLN | A | 293 | 14.242 | 10.156 | 39.972 | 1.00 | 21.37  |
| ATOM | 2220 | CD  | GLN | A | 293 | 12.831 | 9.628  | 39.838 | 1.00 | 24.27  |
| ATOM | 2221 | OE1 | GLN | A | 293 | 12.134 | 9.855  | 38.848 | 1.00 | 23.20  |
| ATOM | 2222 | NE2 | GLN | A | 293 | 12.439 | 8.904  | 40.884 | 1.00 | 18.53  |
| ATOM | 2223 | C   | GLN | A | 293 | 16.816 | 12.029 | 37.805 | 1.00 | 18.20  |
| ATOM | 2224 | O   | GLN | A | 293 | 17.797 | 11.408 | 37.389 | 1.00 | 21.10  |
| ATOM | 2225 | N   | TYR | A | 294 | 16.355 | 13.121 | 37.196 | 1.00 | 20.29  |
| ATOM | 2226 | CA  | TYR | A | 294 | 17.034 | 13.649 | 36.006 | 1.00 | 17.93  |
| ATOM | 2227 | CB  | TYR | A | 294 | 16.239 | 14.824 | 35.456 | 1.00 | 20.72  |
| ATOM | 2228 | CG  | TYR | A | 294 | 16.600 | 15.299 | 34.066 | 1.00 | 22.13  |
| ATOM | 2229 | CD1 | TYR | A | 294 | 16.441 | 14.487 | 32.949 | 1.00 | 22.03  |
| ATOM | 2230 | CE1 | TYR | A | 294 | 16.767 | 14.926 | 31.680 | 1.00 | 27.01  |
| ATOM | 2231 | CZ  | TYR | A | 294 | 17.259 | 16.212 | 31.527 | 1.00 | 31.26  |
| ATOM | 2232 | OH  | TYR | A | 294 | 17.590 | 16.669 | 30.275 | 1.00 | 31.95  |
| ATOM | 2233 | CE2 | TYR | A | 294 | 17.426 | 17.043 | 32.614 | 1.00 | 24.60  |
| ATOM | 2234 | CD2 | TYR | A | 294 | 17.093 | 16.581 | 33.871 | 1.00 | 24.21  |
| ATOM | 2235 | C   | TYR | A | 294 | 18.457 | 14.063 | 36.353 | 1.00 | 26.00  |

**FIGURE 145**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2236 | O   | TYR | A | 294 | 19.401 | 13.726 | 35.643 | 1.00 | 24.45 |
| ATOM | 2237 | N   | VAL | A | 295 | 18.626 | 14.790 | 37.467 | 1.00 | 27.38 |
| ATOM | 2238 | CA  | VAL | A | 295 | 19.981 | 15.130 | 37.908 | 1.00 | 26.38 |
| ATOM | 2239 | CB  | VAL | A | 295 | 19.989 | 15.931 | 39.225 | 1.00 | 21.43 |
| ATOM | 2240 | CG1 | VAL | A | 295 | 21.402 | 15.984 | 39.784 | 1.00 | 28.13 |
| ATOM | 2241 | CG2 | VAL | A | 295 | 19.428 | 17.326 | 39.000 | 1.00 | 34.94 |
| ATOM | 2242 | C   | VAL | A | 295 | 20.839 | 13.888 | 38.136 | 1.00 | 21.34 |
| ATOM | 2243 | O   | VAL | A | 295 | 21.991 | 13.837 | 37.730 | 1.00 | 23.60 |
| ATOM | 2244 | N   | TYR | A | 296 | 20.296 | 12.876 | 38.792 | 1.00 | 22.55 |
| ATOM | 2245 | CA  | TYR | A | 296 | 20.976 | 11.609 | 39.039 | 1.00 | 27.13 |
| ATOM | 2246 | CB  | TYR | A | 296 | 20.011 | 10.665 | 39.773 | 1.00 | 19.15 |
| ATOM | 2247 | CG  | TYR | A | 296 | 20.587 | 9.329  | 40.167 | 1.00 | 22.85 |
| ATOM | 2248 | CD1 | TYR | A | 296 | 21.493 | 9.191  | 41.211 | 1.00 | 21.56 |
| ATOM | 2249 | CE1 | TYR | A | 296 | 22.022 | 7.967  | 41.576 | 1.00 | 20.08 |
| ATOM | 2250 | CZ  | TYR | A | 296 | 21.628 | 6.841  | 40.876 | 1.00 | 22.87 |
| ATOM | 2251 | OH  | TYR | A | 296 | 22.136 | 5.601  | 41.213 | 1.00 | 22.11 |
| ATOM | 2252 | CE2 | TYR | A | 296 | 20.734 | 6.954  | 39.842 | 1.00 | 23.68 |
| ATOM | 2253 | CD2 | TYR | A | 296 | 20.211 | 8.179  | 39.483 | 1.00 | 25.13 |
| ATOM | 2254 | C   | TYR | A | 296 | 21.495 | 10.947 | 37.771 | 1.00 | 22.49 |
| ATOM | 2255 | O   | TYR | A | 296 | 22.607 | 10.406 | 37.752 | 1.00 | 24.52 |
| ATOM | 2256 | N   | LEU | A | 297 | 20.734 | 10.960 | 36.675 | 1.00 | 24.50 |
| ATOM | 2257 | CA  | LEU | A | 297 | 21.265 | 10.390 | 35.437 | 1.00 | 19.36 |
| ATOM | 2258 | CB  | LEU | A | 297 | 20.278 | 10.510 | 34.275 | 1.00 | 22.49 |
| ATOM | 2259 | CG  | LEU | A | 297 | 18.987 | 9.697  | 34.406 | 1.00 | 21.19 |
| ATOM | 2260 | CD1 | LEU | A | 297 | 17.931 | 10.172 | 33.424 | 1.00 | 18.99 |
| ATOM | 2261 | CD2 | LEU | A | 297 | 19.330 | 8.224  | 34.235 | 1.00 | 22.58 |
| ATOM | 2262 | C   | LEU | A | 297 | 22.563 | 11.092 | 35.039 | 1.00 | 22.83 |
| ATOM | 2263 | O   | LEU | A | 297 | 23.545 | 10.455 | 34.672 | 1.00 | 26.28 |
| ATOM | 2264 | N   | HIS | A | 298 | 22.539 | 12.432 | 35.118 | 1.00 | 27.23 |
| ATOM | 2265 | CA  | HIS | A | 298 | 23.760 | 13.165 | 34.773 | 1.00 | 26.75 |
| ATOM | 2266 | CB  | HIS | A | 298 | 23.526 | 14.672 | 34.793 | 1.00 | 25.81 |
| ATOM | 2267 | CG  | HIS | A | 298 | 22.724 | 15.186 | 33.644 | 1.00 | 24.47 |
| ATOM | 2268 | ND1 | HIS | A | 298 | 21.358 | 15.061 | 33.562 | 1.00 | 26.77 |
| ATOM | 2269 | CE1 | HIS | A | 298 | 20.938 | 15.617 | 32.434 | 1.00 | 31.41 |
| ATOM | 2270 | NE2 | HIS | A | 298 | 21.982 | 16.099 | 31.780 | 1.00 | 22.95 |
| ATOM | 2271 | CD2 | HIS | A | 298 | 23.105 | 15.841 | 32.519 | 1.00 | 26.28 |
| ATOM | 2272 | C   | HIS | A | 298 | 24.877 | 12.814 | 35.749 | 1.00 | 24.86 |
| ATOM | 2273 | O   | HIS | A | 298 | 26.009 | 12.584 | 35.342 | 1.00 | 32.20 |
| ATOM | 2274 | N   | GLN | A | 299 | 24.555 | 12.775 | 37.044 | 1.00 | 20.61 |
| ATOM | 2275 | CA  | GLN | A | 299 | 25.600 | 12.405 | 38.005 | 1.00 | 27.30 |
| ATOM | 2276 | CB  | GLN | A | 299 | 25.077 | 12.420 | 39.440 | 1.00 | 29.89 |
| ATOM | 2277 | CG  | GLN | A | 299 | 24.644 | 13.789 | 39.945 | 1.00 | 29.83 |
| ATOM | 2278 | CD  | GLN | A | 299 | 24.030 | 13.768 | 41.327 | 1.00 | 39.67 |
| ATOM | 2279 | OE1 | GLN | A | 299 | 23.233 | 12.894 | 41.678 | 1.00 | 50.54 |
| ATOM | 2280 | NE2 | GLN | A | 299 | 24.382 | 14.755 | 42.148 | 1.00 | 42.66 |
| ATOM | 2281 | C   | GLN | A | 299 | 26.174 | 11.033 | 37.665 | 1.00 | 30.62 |
| ATOM | 2282 | O   | GLN | A | 299 | 27.380 | 10.808 | 37.781 | 1.00 | 24.65 |
| ATOM | 2283 | N   | CYS | A | 300 | 25.311 | 10.110 | 37.244 | 1.00 | 32.98 |
| ATOM | 2284 | CA  | CYS | A | 300 | 25.750 | 8.773  | 36.865 | 1.00 | 31.19 |
| ATOM | 2285 | CB  | CYS | A | 300 | 24.539 | 7.921  | 36.453 | 1.00 | 27.79 |
| ATOM | 2286 | SG  | CYS | A | 300 | 23.647 | 7.209  | 37.864 | 1.00 | 24.58 |
| ATOM | 2287 | C   | CYS | A | 300 | 26.765 | 8.828  | 35.727 | 1.00 | 34.76 |

**FIGURE 146**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2288 | O   | CYS | A | 300 | 27.822 | 8.196  | 35.729 | 1.00 | 23.29 |
| ATOM | 2289 | N   | VAL | A | 301 | 26.420 | 9.615  | 34.708 | 1.00 | 32.86 |
| ATOM | 2290 | CA  | VAL | A | 301 | 27.302 | 9.758  | 33.561 | 1.00 | 33.82 |
| ATOM | 2291 | CB  | VAL | A | 301 | 26.630 | 10.582 | 32.444 | 1.00 | 31.77 |
| ATOM | 2292 | CG1 | VAL | A | 301 | 27.618 | 10.894 | 31.330 | 1.00 | 32.91 |
| ATOM | 2293 | CG2 | VAL | A | 301 | 25.418 | 9.821  | 31.923 | 1.00 | 36.31 |
| ATOM | 2294 | C   | VAL | A | 301 | 28.618 | 10.429 | 33.941 | 1.00 | 30.73 |
| ATOM | 2295 | O   | VAL | A | 301 | 29.692 | 10.022 | 33.501 | 1.00 | 35.82 |
| ATOM | 2296 | N   | ARG | A | 302 | 28.541 | 11.468 | 34.763 | 1.00 | 31.17 |
| ATOM | 2297 | CA  | ARG | A | 302 | 29.790 | 12.172 | 35.086 | 1.00 | 30.26 |
| ATOM | 2298 | CB  | ARG | A | 302 | 29.484 | 13.422 | 35.894 | 1.00 | 32.62 |
| ATOM | 2299 | CG  | ARG | A | 302 | 30.689 | 14.073 | 36.564 | 1.00 | 30.76 |
| ATOM | 2300 | CD  | ARG | A | 302 | 30.203 | 14.793 | 37.826 | 1.00 | 35.56 |
| ATOM | 2301 | NE  | ARG | A | 302 | 29.679 | 13.851 | 38.796 | 1.00 | 36.12 |
| ATOM | 2302 | CZ  | ARG | A | 302 | 28.999 | 14.106 | 39.898 | 1.00 | 43.20 |
| ATOM | 2303 | NH1 | ARG | A | 302 | 28.702 | 15.351 | 40.255 | 1.00 | 58.84 |
| ATOM | 2304 | NH2 | ARG | A | 302 | 28.601 | 13.098 | 40.671 | 1.00 | 37.42 |
| ATOM | 2305 | C   | ARG | A | 302 | 30.720 | 11.213 | 35.811 | 1.00 | 38.00 |
| ATOM | 2306 | O   | ARG | A | 302 | 31.934 | 11.187 | 35.602 | 1.00 | 46.79 |
| ATOM | 2307 | N   | ASP | A | 303 | 30.137 | 10.376 | 36.668 | 1.00 | 34.78 |
| ATOM | 2308 | CA  | ASP | A | 303 | 30.980 | 9.431  | 37.404 | 1.00 | 31.64 |
| ATOM | 2309 | CB  | ASP | A | 303 | 30.186 | 8.844  | 38.579 | 1.00 | 32.29 |
| ATOM | 2310 | CG  | ASP | A | 303 | 29.766 | 9.934  | 39.553 | 1.00 | 41.64 |
| ATOM | 2311 | OD1 | ASP | A | 303 | 30.143 | 11.104 | 39.315 | 1.00 | 48.79 |
| ATOM | 2312 | OD2 | ASP | A | 303 | 29.060 | 9.645  | 40.542 | 1.00 | 39.40 |
| ATOM | 2313 | C   | ASP | A | 303 | 31.529 | 8.359  | 36.484 | 1.00 | 33.95 |
| ATOM | 2314 | O   | ASP | A | 303 | 32.681 | 7.925  | 36.612 | 1.00 | 41.56 |
| ATOM | 2315 | N   | VAL | A | 304 | 30.755 | 7.875  | 35.510 | 1.00 | 31.21 |
| ATOM | 2316 | CA  | VAL | A | 304 | 31.349 | 6.840  | 34.658 | 1.00 | 39.08 |
| ATOM | 2317 | CB  | VAL | A | 304 | 30.371 | 6.167  | 33.685 | 1.00 | 44.47 |
| ATOM | 2318 | CG1 | VAL | A | 304 | 31.089 | 5.084  | 32.889 | 1.00 | 27.60 |
| ATOM | 2319 | CG2 | VAL | A | 304 | 29.173 | 5.541  | 34.381 | 1.00 | 27.78 |
| ATOM | 2320 | C   | VAL | A | 304 | 32.485 | 7.483  | 33.859 | 1.00 | 39.60 |
| ATOM | 2321 | O   | VAL | A | 304 | 33.515 | 6.865  | 33.615 | 1.00 | 37.42 |
| ATOM | 2322 | N   | LEU | A | 305 | 32.257 | 8.736  | 33.484 | 1.00 | 36.24 |
| ATOM | 2323 | CA  | LEU | A | 305 | 33.241 | 9.491  | 32.714 | 1.00 | 42.98 |
| ATOM | 2324 | CB  | LEU | A | 305 | 32.620 | 10.746 | 32.093 | 1.00 | 39.34 |
| ATOM | 2325 | CG  | LEU | A | 305 | 31.658 | 10.512 | 30.929 | 1.00 | 34.01 |
| ATOM | 2326 | CD1 | LEU | A | 305 | 31.183 | 11.828 | 30.327 | 1.00 | 28.76 |
| ATOM | 2327 | CD2 | LEU | A | 305 | 32.315 | 9.625  | 29.876 | 1.00 | 34.10 |
| ATOM | 2328 | C   | LEU | A | 305 | 34.425 | 9.863  | 33.598 | 1.00 | 42.82 |
| ATOM | 2329 | O   | LEU | A | 305 | 35.578 | 9.705  | 33.198 | 1.00 | 54.32 |
| ATOM | 2330 | N   | ARG | A | 306 | 34.150 | 10.353 | 34.805 | 1.00 | 41.87 |
| ATOM | 2331 | CA  | ARG | A | 306 | 35.253 | 10.741 | 35.681 | 1.00 | 51.42 |
| ATOM | 2332 | CB  | ARG | A | 306 | 34.725 | 11.361 | 36.979 | 1.00 | 50.76 |
| ATOM | 2333 | CG  | ARG | A | 306 | 34.163 | 12.761 | 36.809 | 1.00 | 57.18 |
| ATOM | 2334 | CD  | ARG | A | 306 | 33.547 | 13.297 | 38.093 | 1.00 | 63.89 |
| ATOM | 2335 | NE  | ARG | A | 306 | 33.871 | 14.701 | 38.302 | 1.00 | 65.68 |
| ATOM | 2336 | CZ  | ARG | A | 306 | 33.491 | 15.494 | 39.287 | 1.00 | 66.42 |
| ATOM | 2337 | NH1 | ARG | A | 306 | 32.710 | 15.080 | 40.276 | 1.00 | 39.94 |
| ATOM | 2338 | NH2 | ARG | A | 306 | 33.906 | 16.759 | 39.290 | 1.00 | 95.50 |
| ATOM | 2339 | C   | ARG | A | 306 | 36.161 | 9.553  | 35.988 | 1.00 | 65.39 |

**FIGURE 147**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2340 | O   | ARG | A | 306 | 37.371 | 9.710  | 36.183 | 1.00 | 79.48 |
| ATOM | 2341 | N   | ALA | A | 307 | 35.593 | 8.350  | 36.039 | 1.00 | 63.13 |
| ATOM | 2342 | CA  | ALA | A | 307 | 36.358 | 7.181  | 36.463 | 1.00 | 59.88 |
| ATOM | 2343 | CB  | ALA | A | 307 | 35.424 | 6.123  | 37.032 | 1.00 | 62.57 |
| ATOM | 2344 | C   | ALA | A | 307 | 37.190 | 6.603  | 35.327 | 1.00 | 63.48 |
| ATOM | 2345 | O   | ALA | A | 307 | 38.185 | 5.922  | 35.576 | 1.00 | 71.07 |
| ATOM | 2346 | N   | ARG | A | 308 | 36.778 | 6.878  | 34.095 | 1.00 | 66.80 |
| ATOM | 2347 | CA  | ARG | A | 308 | 37.460 | 6.357  | 32.916 | 1.00 | 63.53 |
| ATOM | 2348 | CB  | ARG | A | 308 | 36.431 | 5.843  | 31.910 | 1.00 | 64.58 |
| ATOM | 2349 | CG  | ARG | A | 308 | 35.909 | 6.905  | 30.956 | 1.00 | 73.99 |
| ATOM | 2350 | CD  | ARG | A | 308 | 34.390 | 6.946  | 30.959 | 1.00 | 81.85 |
| ATOM | 2351 | NE  | ARG | A | 308 | 33.814 | 5.939  | 30.070 | 1.00 | 85.42 |
| ATOM | 2352 | CZ  | ARG | A | 308 | 33.523 | 6.167  | 28.794 | 1.00 | 82.34 |
| ATOM | 2353 | NH1 | ARG | A | 308 | 33.757 | 7.365  | 28.275 | 1.00 | 72.00 |
| ATOM | 2354 | NH2 | ARG | A | 308 | 33.001 | 5.198  | 28.053 | 1.00 | 74.84 |
| ATOM | 2355 | C   | ARG | A | 308 | 38.356 | 7.408  | 32.272 | 1.00 | 66.32 |
| ATOM | 2356 | O   | ARG | A | 308 | 39.461 | 7.117  | 31.813 | 1.00 | 55.04 |
| ATOM | 2357 | N   | THR | B | 20  | 44.023 | 9.553  | 52.894 | 1.00 | 44.19 |
| ATOM | 2358 | CA  | THR | B | 20  | 43.083 | 8.735  | 53.658 | 1.00 | 52.64 |
| ATOM | 2359 | CB  | THR | B | 20  | 43.790 | 7.980  | 54.795 | 1.00 | 59.51 |
| ATOM | 2360 | OG1 | THR | B | 20  | 45.173 | 7.808  | 54.450 | 1.00 | 74.31 |
| ATOM | 2361 | CG2 | THR | B | 20  | 43.208 | 6.590  | 54.985 | 1.00 | 67.07 |
| ATOM | 2362 | C   | THR | B | 20  | 41.947 | 9.580  | 54.229 | 1.00 | 46.00 |
| ATOM | 2363 | O   | THR | B | 20  | 42.162 | 10.580 | 54.911 | 1.00 | 47.42 |
| ATOM | 2364 | N   | SER | B | 21  | 40.725 | 9.158  | 53.926 | 1.00 | 41.46 |
| ATOM | 2365 | CA  | SER | B | 21  | 39.496 | 9.819  | 54.320 | 1.00 | 39.05 |
| ATOM | 2366 | CB  | SER | B | 21  | 39.040 | 10.796 | 53.232 | 1.00 | 49.38 |
| ATOM | 2367 | OG  | SER | B | 21  | 37.654 | 10.651 | 52.968 | 1.00 | 64.42 |
| ATOM | 2368 | C   | SER | B | 21  | 38.381 | 8.816  | 54.580 | 1.00 | 45.97 |
| ATOM | 2369 | O   | SER | B | 21  | 38.392 | 7.690  | 54.078 | 1.00 | 58.15 |
| ATOM | 2370 | N   | CYS | B | 22  | 37.384 | 9.218  | 55.363 | 1.00 | 49.85 |
| ATOM | 2371 | CA  | CYS | B | 22  | 36.237 | 8.334  | 55.572 | 1.00 | 50.77 |
| ATOM | 2372 | CB  | CYS | B | 22  | 36.423 | 7.465  | 56.816 | 1.00 | 55.65 |
| ATOM | 2373 | SG  | CYS | B | 22  | 35.067 | 6.307  | 57.123 | 1.00 | 88.47 |
| ATOM | 2374 | C   | CYS | B | 22  | 34.951 | 9.143  | 55.677 | 1.00 | 45.29 |
| ATOM | 2375 | O   | CYS | B | 22  | 34.411 | 9.331  | 56.767 | 1.00 | 58.34 |
| ATOM | 2376 | N   | PRO | B | 23  | 34.467 | 9.632  | 54.543 | 1.00 | 39.55 |
| ATOM | 2377 | CA  | PRO | B | 23  | 33.212 | 10.389 | 54.528 | 1.00 | 41.51 |
| ATOM | 2378 | CB  | PRO | B | 23  | 33.049 | 10.758 | 53.050 | 1.00 | 40.09 |
| ATOM | 2379 | CG  | PRO | B | 23  | 34.441 | 10.713 | 52.503 | 1.00 | 41.78 |
| ATOM | 2380 | CD  | PRO | B | 23  | 35.072 | 9.531  | 53.203 | 1.00 | 44.99 |
| ATOM | 2381 | C   | PRO | B | 23  | 32.027 | 9.552  | 55.000 | 1.00 | 44.21 |
| ATOM | 2382 | O   | PRO | B | 23  | 31.963 | 8.335  | 54.814 | 1.00 | 52.40 |
| ATOM | 2383 | N   | ILE | B | 24  | 31.065 | 10.223 | 55.624 | 1.00 | 44.34 |
| ATOM | 2384 | CA  | ILE | B | 24  | 29.827 | 9.587  | 56.044 | 1.00 | 48.20 |
| ATOM | 2385 | CB  | ILE | B | 24  | 29.721 | 9.319  | 57.555 | 1.00 | 45.03 |
| ATOM | 2386 | CG1 | ILE | B | 24  | 31.043 | 9.095  | 58.282 | 1.00 | 44.77 |
| ATOM | 2387 | CD1 | ILE | B | 24  | 31.305 | 10.113 | 59.373 | 1.00 | 61.25 |
| ATOM | 2388 | CG2 | ILE | B | 24  | 28.778 | 8.151  | 57.813 | 1.00 | 56.04 |
| ATOM | 2389 | C   | ILE | B | 24  | 28.646 | 10.483 | 55.663 | 1.00 | 48.34 |
| ATOM | 2390 | O   | ILE | B | 24  | 28.590 | 11.626 | 56.128 | 1.00 | 36.96 |
| ATOM | 2391 | N   | LYS | B | 25  | 27.747 | 9.948  | 54.848 | 1.00 | 44.27 |

**FIGURE 148**



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2392 | CA  | LYS | B | 25 | 26.540 | 10.698 | 54.492 | 1.00 | 52.98 |
| ATOM | 2393 | CB  | LYS | B | 25 | 25.594 | 9.846  | 53.655 | 1.00 | 62.63 |
| ATOM | 2394 | CG  | LYS | B | 25 | 25.908 | 9.737  | 52.176 | 1.00 | 62.43 |
| ATOM | 2395 | CD  | LYS | B | 25 | 27.378 | 9.486  | 51.908 | 1.00 | 63.27 |
| ATOM | 2396 | CE  | LYS | B | 25 | 27.772 | 8.047  | 52.197 | 1.00 | 62.30 |
| ATOM | 2397 | NZ  | LYS | B | 25 | 29.243 | 7.842  | 52.072 | 1.00 | 60.67 |
| ATOM | 2398 | C   | LYS | B | 25 | 25.859 | 11.181 | 55.772 | 1.00 | 48.94 |
| ATOM | 2399 | O   | LYS | B | 25 | 25.679 | 10.387 | 56.698 | 1.00 | 46.18 |
| ATOM | 2400 | N   | ILE | B | 26 | 25.523 | 12.466 | 55.828 | 1.00 | 51.90 |
| ATOM | 2401 | CA  | ILE | B | 26 | 24.977 | 13.025 | 57.066 | 1.00 | 54.24 |
| ATOM | 2402 | CB  | ILE | B | 26 | 24.660 | 14.523 | 56.951 | 1.00 | 63.05 |
| ATOM | 2403 | CG1 | ILE | B | 26 | 23.589 | 14.879 | 55.916 | 1.00 | 68.15 |
| ATOM | 2404 | CD1 | ILE | B | 26 | 22.545 | 15.837 | 56.460 | 1.00 | 71.59 |
| ATOM | 2405 | CG2 | ILE | B | 26 | 25.929 | 15.325 | 56.685 | 1.00 | 65.12 |
| ATOM | 2406 | C   | ILE | B | 26 | 23.733 | 12.241 | 57.465 | 1.00 | 51.02 |
| ATOM | 2407 | O   | ILE | B | 26 | 23.573 | 11.830 | 58.614 | 1.00 | 47.65 |
| ATOM | 2408 | N   | ASN | B | 27 | 22.870 | 12.003 | 56.483 | 1.00 | 51.44 |
| ATOM | 2409 | CA  | ASN | B | 27 | 21.666 | 11.219 | 56.721 | 1.00 | 61.45 |
| ATOM | 2410 | CB  | ASN | B | 27 | 20.899 | 10.993 | 55.415 | 1.00 | 75.84 |
| ATOM | 2411 | CG  | ASN | B | 27 | 20.870 | 12.209 | 54.511 | 1.00 | 85.31 |
| ATOM | 2412 | OD1 | ASN | B | 27 | 21.910 | 12.672 | 54.041 | 1.00 | 99.97 |
| ATOM | 2413 | ND2 | ASN | B | 27 | 19.672 | 12.729 | 54.262 | 1.00 | 93.77 |
| ATOM | 2414 | C   | ASN | B | 27 | 21.985 | 9.885  | 57.379 | 1.00 | 55.35 |
| ATOM | 2415 | O   | ASN | B | 27 | 21.135 | 9.336  | 58.089 | 1.00 | 88.25 |
| ATOM | 2416 | N   | GLN | B | 28 | 23.176 | 9.311  | 57.195 | 1.00 | 48.45 |
| ATOM | 2417 | CA  | GLN | B | 28 | 23.415 | 8.047  | 57.894 | 1.00 | 52.09 |
| ATOM | 2418 | CB  | GLN | B | 28 | 24.024 | 6.974  | 56.990 | 1.00 | 57.63 |
| ATOM | 2419 | CG  | GLN | B | 28 | 24.654 | 7.430  | 55.694 | 1.00 | 63.93 |
| ATOM | 2420 | CD  | GLN | B | 28 | 24.174 | 6.638  | 54.490 | 1.00 | 71.84 |
| ATOM | 2421 | OE1 | GLN | B | 28 | 24.797 | 5.657  | 54.074 | 1.00 | 79.09 |
| ATOM | 2422 | NE2 | GLN | B | 28 | 23.051 | 7.067  | 53.920 | 1.00 | 63.99 |
| ATOM | 2423 | C   | GLN | B | 28 | 24.321 | 8.227  | 59.103 | 1.00 | 48.62 |
| ATOM | 2424 | O   | GLN | B | 28 | 24.763 | 7.214  | 59.654 | 1.00 | 48.29 |
| ATOM | 2425 | N   | PHE | B | 29 | 24.617 | 9.452  | 59.529 | 1.00 | 55.12 |
| ATOM | 2426 | CA  | PHE | B | 29 | 25.569 | 9.586  | 60.626 | 1.00 | 55.39 |
| ATOM | 2427 | CB  | PHE | B | 29 | 25.852 | 11.055 | 61.000 | 1.00 | 55.09 |
| ATOM | 2428 | CG  | PHE | B | 29 | 27.126 | 11.084 | 61.852 | 1.00 | 51.70 |
| ATOM | 2429 | CD1 | PHE | B | 29 | 28.363 | 11.038 | 61.233 | 1.00 | 54.80 |
| ATOM | 2430 | CE1 | PHE | B | 29 | 29.521 | 11.046 | 61.984 | 1.00 | 57.30 |
| ATOM | 2431 | CZ  | PHE | B | 29 | 29.458 | 11.100 | 63.365 | 1.00 | 54.61 |
| ATOM | 2432 | CE2 | PHE | B | 29 | 28.227 | 11.150 | 63.988 | 1.00 | 44.82 |
| ATOM | 2433 | CD2 | PHE | B | 29 | 27.071 | 11.145 | 63.230 | 1.00 | 41.09 |
| ATOM | 2434 | C   | PHE | B | 29 | 25.123 | 8.850  | 61.890 | 1.00 | 57.59 |
| ATOM | 2435 | O   | PHE | B | 29 | 25.964 | 8.281  | 62.594 | 1.00 | 47.92 |
| ATOM | 2436 | N   | GLU | B | 30 | 23.828 | 8.867  | 62.167 | 1.00 | 63.38 |
| ATOM | 2437 | CA  | GLU | B | 30 | 23.280 | 8.207  | 63.344 | 1.00 | 62.77 |
| ATOM | 2438 | CB  | GLU | B | 30 | 21.748 | 8.203  | 63.264 | 1.00 | 73.02 |
| ATOM | 2439 | CG  | GLU | B | 30 | 21.122 | 9.397  | 63.971 | 1.00 | 77.36 |
| ATOM | 2440 | CD  | GLU | B | 30 | 21.462 | 9.438  | 65.448 | 1.00 | 78.77 |
| ATOM | 2441 | OE1 | GLU | B | 30 | 20.929 | 10.329 | 66.141 | 1.00 | 79.79 |
| ATOM | 2442 | OE2 | GLU | B | 30 | 22.251 | 8.592  | 65.918 | 1.00 | 84.00 |
| ATOM | 2443 | C   | GLU | B | 30 | 23.793 | 6.783  | 63.519 | 1.00 | 54.87 |

**FIGURE 149**

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2444 | O   | GLU | B | 30 | 24.369 | 6.475  | 64.563 | 1.00 | 35.09 |
| ATOM | 2445 | N   | GLY | B | 31 | 23.595 | 5.938  | 62.517 | 1.00 | 59.10 |
| ATOM | 2446 | CA  | GLY | B | 31 | 23.994 | 4.545  | 62.525 | 1.00 | 56.95 |
| ATOM | 2447 | C   | GLY | B | 31 | 25.493 | 4.331  | 62.443 | 1.00 | 59.39 |
| ATOM | 2448 | O   | GLY | B | 31 | 26.019 | 3.379  | 63.037 | 1.00 | 42.38 |
| ATOM | 2449 | N   | HIS | B | 32 | 26.167 | 5.215  | 61.710 | 1.00 | 59.10 |
| ATOM | 2450 | CA  | HIS | B | 32 | 27.629 | 5.216  | 61.649 | 1.00 | 51.48 |
| ATOM | 2451 | CB  | HIS | B | 32 | 28.127 | 6.437  | 60.888 | 1.00 | 51.68 |
| ATOM | 2452 | CG  | HIS | B | 32 | 29.593 | 6.534  | 60.618 | 1.00 | 64.14 |
| ATOM | 2453 | ND1 | HIS | B | 32 | 30.445 | 7.321  | 61.368 | 1.00 | 66.96 |
| ATOM | 2454 | CE1 | HIS | B | 32 | 31.680 | 7.223  | 60.917 | 1.00 | 64.66 |
| ATOM | 2455 | NE2 | HIS | B | 32 | 31.669 | 6.399  | 59.884 | 1.00 | 69.62 |
| ATOM | 2456 | CD2 | HIS | B | 32 | 30.382 | 5.959  | 59.681 | 1.00 | 69.44 |
| ATOM | 2457 | C   | HIS | B | 32 | 28.174 | 5.164  | 63.071 | 1.00 | 48.27 |
| ATOM | 2458 | O   | HIS | B | 32 | 28.812 | 4.198  | 63.493 | 1.00 | 43.02 |
| ATOM | 2459 | N   | PHE | B | 33 | 27.893 | 6.215  | 63.836 | 1.00 | 52.78 |
| ATOM | 2460 | CA  | PHE | B | 33 | 28.398 | 6.300  | 65.205 | 1.00 | 56.25 |
| ATOM | 2461 | CB  | PHE | B | 33 | 27.898 | 7.596  | 65.853 | 1.00 | 58.42 |
| ATOM | 2462 | CG  | PHE | B | 33 | 28.693 | 8.008  | 67.083 | 1.00 | 52.11 |
| ATOM | 2463 | CD1 | PHE | B | 33 | 30.015 | 7.634  | 67.229 | 1.00 | 40.98 |
| ATOM | 2464 | CE1 | PHE | B | 33 | 30.727 | 8.001  | 68.354 | 1.00 | 46.43 |
| ATOM | 2465 | CZ  | PHE | B | 33 | 30.127 | 8.753  | 69.348 | 1.00 | 46.14 |
| ATOM | 2466 | CE2 | PHE | B | 33 | 28.806 | 9.135  | 69.208 | 1.00 | 46.50 |
| ATOM | 2467 | CD2 | PHE | B | 33 | 28.101 | 8.767  | 68.079 | 1.00 | 53.38 |
| ATOM | 2468 | C   | PHE | B | 33 | 28.022 | 5.075  | 66.032 | 1.00 | 55.13 |
| ATOM | 2469 | O   | PHE | B | 33 | 28.890 | 4.473  | 66.675 | 1.00 | 37.79 |
| ATOM | 2470 | N   | MET | B | 34 | 26.755 | 4.681  | 66.032 | 1.00 | 65.84 |
| ATOM | 2471 | CA  | MET | B | 34 | 26.316 | 3.484  | 66.751 | 1.00 | 75.38 |
| ATOM | 2472 | CB  | MET | B | 34 | 24.841 | 3.195  | 66.464 | 1.00 | 80.09 |
| ATOM | 2473 | CG  | MET | B | 34 | 23.886 | 3.798  | 67.480 | 1.00 | 84.30 |
| ATOM | 2474 | SD  | MET | B | 34 | 22.339 | 4.405  | 66.779 | 1.00 | 87.53 |
| ATOM | 2475 | CE  | MET | B | 34 | 21.767 | 2.952  | 65.905 | 1.00 | 52.16 |
| ATOM | 2476 | C   | MET | B | 34 | 27.188 | 2.284  | 66.383 | 1.00 | 75.48 |
| ATOM | 2477 | O   | MET | B | 34 | 27.588 | 1.495  | 67.238 | 1.00 | 66.38 |
| ATOM | 2478 | N   | LYS | B | 35 | 27.503 | 2.192  | 65.096 | 1.00 | 75.62 |
| ATOM | 2479 | CA  | LYS | B | 35 | 28.410 | 1.192  | 64.561 | 1.00 | 70.36 |
| ATOM | 2480 | CB  | LYS | B | 35 | 28.646 | 1.437  | 63.066 | 1.00 | 73.89 |
| ATOM | 2481 | CG  | LYS | B | 35 | 27.460 | 1.150  | 62.169 | 1.00 | 77.64 |
| ATOM | 2482 | CD  | LYS | B | 35 | 27.860 | 0.247  | 61.008 | 1.00 | 79.39 |
| ATOM | 2483 | CE  | LYS | B | 35 | 27.676 | -1.218 | 61.371 | 1.00 | 81.96 |
| ATOM | 2484 | NZ  | LYS | B | 35 | 28.542 | -1.629 | 62.510 | 1.00 | 89.41 |
| ATOM | 2485 | C   | LYS | B | 35 | 29.760 | 1.199  | 65.265 | 1.00 | 64.44 |
| ATOM | 2486 | O   | LYS | B | 35 | 30.185 | 0.235  | 65.901 | 1.00 | 37.91 |
| ATOM | 2487 | N   | LEU | B | 36 | 30.485 | 2.316  | 65.147 | 1.00 | 63.16 |
| ATOM | 2488 | CA  | LEU | B | 36 | 31.841 | 2.334  | 65.693 | 1.00 | 63.09 |
| ATOM | 2489 | CB  | LEU | B | 36 | 32.573 | 3.624  | 65.324 | 1.00 | 65.24 |
| ATOM | 2490 | CG  | LEU | B | 36 | 32.842 | 3.848  | 63.836 | 1.00 | 68.40 |
| ATOM | 2491 | CD1 | LEU | B | 36 | 31.931 | 4.933  | 63.279 | 1.00 | 66.79 |
| ATOM | 2492 | CD2 | LEU | B | 36 | 34.303 | 4.199  | 63.599 | 1.00 | 81.44 |
| ATOM | 2493 | C   | LEU | B | 36 | 31.826 | 2.156  | 67.209 | 1.00 | 56.96 |
| ATOM | 2494 | O   | LEU | B | 36 | 32.833 | 1.728  | 67.774 | 1.00 | 56.27 |
| ATOM | 2495 | N   | GLN | B | 37 | 30.691 | 2.487  | 67.805 | 1.00 | 53.43 |

FIGURE 150

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2496 | CA  | GLN | B | 37 | 30.459 | 2.414  | 69.236 | 1.00 | 69.43 |
| ATOM | 2497 | CB  | GLN | B | 37 | 29.331 | 3.386  | 69.619 | 1.00 | 68.76 |
| ATOM | 2498 | CG  | GLN | B | 37 | 29.831 | 4.826  | 69.657 | 1.00 | 75.93 |
| ATOM | 2499 | CD  | GLN | B | 37 | 28.722 | 5.824  | 69.917 | 1.00 | 77.13 |
| ATOM | 2500 | OE1 | GLN | B | 37 | 27.936 | 6.137  | 69.020 | 1.00 | 87.89 |
| ATOM | 2501 | NE2 | GLN | B | 37 | 28.671 | 6.319  | 71.147 | 1.00 | 60.96 |
| ATOM | 2502 | C   | GLN | B | 37 | 30.117 | 1.006  | 69.706 | 1.00 | 79.22 |
| ATOM | 2503 | O   | GLN | B | 37 | 30.388 | 0.635  | 70.850 | 1.00 | 73.11 |
| ATOM | 2504 | N   | ALA | B | 38 | 29.518 | 0.228  | 68.808 | 1.00 | 83.91 |
| ATOM | 2505 | CA  | ALA | B | 38 | 29.154 | -1.148 | 69.119 | 1.00 | 85.90 |
| ATOM | 2506 | CB  | ALA | B | 38 | 28.533 | -1.809 | 67.896 | 1.00 | 73.44 |
| ATOM | 2507 | C   | ALA | B | 38 | 30.354 | -1.952 | 69.612 | 1.00 | 87.80 |
| ATOM | 2508 | O   | ALA | B | 38 | 31.504 | -1.707 | 69.247 | 1.00 | 77.48 |
| ATOM | 2509 | N   | ASP | B | 39 | 30.073 | -2.936 | 70.462 | 1.00 | 88.62 |
| ATOM | 2510 | CA  | ASP | B | 39 | 31.113 | -3.821 | 70.969 | 1.00 | 85.89 |
| ATOM | 2511 | CB  | ASP | B | 39 | 31.626 | -4.719 | 69.837 | 1.00 | 87.42 |
| ATOM | 2512 | CG  | ASP | B | 39 | 30.689 | -5.885 | 69.586 | 1.00 | 90.49 |
| ATOM | 2513 | OD1 | ASP | B | 39 | 30.455 | -6.223 | 68.408 | 1.00 | 97.09 |
| ATOM | 2514 | OD2 | ASP | B | 39 | 30.188 | -6.455 | 70.579 | 1.00 | 93.16 |
| ATOM | 2515 | C   | ASP | B | 39 | 32.267 | -3.044 | 71.587 | 1.00 | 82.50 |
| ATOM | 2516 | O   | ASP | B | 39 | 33.429 | -3.298 | 71.271 | 1.00 | 76.36 |
| ATOM | 2517 | N   | SER | B | 40 | 31.940 | -2.102 | 72.465 | 1.00 | 82.73 |
| ATOM | 2518 | CA  | SER | B | 40 | 32.957 | -1.326 | 73.165 | 1.00 | 79.40 |
| ATOM | 2519 | CB  | SER | B | 40 | 33.839 | -2.246 | 74.009 | 1.00 | 75.80 |
| ATOM | 2520 | OG  | SER | B | 40 | 34.651 | -3.081 | 73.205 | 1.00 | 54.94 |
| ATOM | 2521 | C   | SER | B | 40 | 33.807 | -0.518 | 72.180 | 1.00 | 76.46 |
| ATOM | 2522 | O   | SER | B | 40 | 35.024 | -0.714 | 72.131 | 1.00 | 64.01 |
| ATOM | 2523 | N   | ASN | B | 41 | 33.121 | 0.352  | 71.454 | 1.00 | 73.19 |
| ATOM | 2524 | CA  | ASN | B | 41 | 33.647 | 1.191  | 70.394 | 1.00 | 71.55 |
| ATOM | 2525 | CB  | ASN | B | 41 | 34.253 | 2.492  | 70.912 | 1.00 | 67.00 |
| ATOM | 2526 | CG  | ASN | B | 41 | 33.360 | 3.337  | 71.784 | 1.00 | 65.98 |
| ATOM | 2527 | OD1 | ASN | B | 41 | 32.134 | 3.225  | 71.788 | 1.00 | 77.13 |
| ATOM | 2528 | ND2 | ASN | B | 41 | 33.976 | 4.224  | 72.563 | 1.00 | 62.14 |
| ATOM | 2529 | C   | ASN | B | 41 | 34.710 | 0.429  | 69.603 | 1.00 | 74.40 |
| ATOM | 2530 | O   | ASN | B | 41 | 35.806 | 0.941  | 69.376 | 1.00 | 81.24 |
| ATOM | 2531 | N   | TYR | B | 42 | 34.393 | -0.804 | 69.212 | 1.00 | 74.86 |
| ATOM | 2532 | CA  | TYR | B | 42 | 35.405 | -1.610 | 68.534 | 1.00 | 74.76 |
| ATOM | 2533 | CB  | TYR | B | 42 | 34.880 | -3.002 | 68.168 | 1.00 | 75.15 |
| ATOM | 2534 | CG  | TYR | B | 42 | 35.907 | -3.795 | 67.386 | 1.00 | 75.66 |
| ATOM | 2535 | CD1 | TYR | B | 42 | 37.017 | -4.332 | 68.023 | 1.00 | 78.98 |
| ATOM | 2536 | CE1 | TYR | B | 42 | 37.961 | -5.054 | 67.316 | 1.00 | 81.79 |
| ATOM | 2537 | CZ  | TYR | B | 42 | 37.804 | -5.243 | 65.959 | 1.00 | 81.37 |
| ATOM | 2538 | OH  | TYR | B | 42 | 38.747 | -5.962 | 65.258 | 1.00 | 80.99 |
| ATOM | 2539 | CE2 | TYR | B | 42 | 36.713 | -4.717 | 65.304 | 1.00 | 76.53 |
| ATOM | 2540 | CD2 | TYR | B | 42 | 35.775 | -3.996 | 66.019 | 1.00 | 75.88 |
| ATOM | 2541 | C   | TYR | B | 42 | 35.914 | -0.906 | 67.277 | 1.00 | 72.94 |
| ATOM | 2542 | O   | TYR | B | 42 | 37.119 | -0.676 | 67.155 | 1.00 | 61.94 |
| ATOM | 2543 | N   | LEU | B | 43 | 35.004 | -0.570 | 66.366 | 1.00 | 68.88 |
| ATOM | 2544 | CA  | LEU | B | 43 | 35.396 | 0.092  | 65.128 | 1.00 | 70.56 |
| ATOM | 2545 | CB  | LEU | B | 43 | 34.188 | 0.493  | 64.286 | 1.00 | 72.58 |
| ATOM | 2546 | CG  | LEU | B | 43 | 33.017 | -0.487 | 64.224 | 1.00 | 76.87 |
| ATOM | 2547 | CD1 | LEU | B | 43 | 31.993 | -0.053 | 63.184 | 1.00 | 62.51 |

**FIGURE 151**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2548 | CD2 | LEU | B | 43 | 33.520 | -1.895 | 63.937 | 1.00 | 77.97 |
| ATOM | 2549 | C   | LEU | B | 43 | 36.248 | 1.336  | 65.417 | 1.00 | 67.14 |
| ATOM | 2550 | O   | LEU | B | 43 | 37.449 | 1.316  | 65.140 | 1.00 | 50.41 |
| ATOM | 2551 | N   | LEU | B | 44 | 35.580 | 2.345  | 65.951 | 1.00 | 66.03 |
| ATOM | 2552 | CA  | LEU | B | 44 | 36.109 | 3.651  | 66.304 | 1.00 | 61.62 |
| ATOM | 2553 | CB  | LEU | B | 44 | 35.238 | 4.313  | 67.375 | 1.00 | 62.58 |
| ATOM | 2554 | CG  | LEU | B | 44 | 35.741 | 5.640  | 67.946 | 1.00 | 58.19 |
| ATOM | 2555 | CD1 | LEU | B | 44 | 34.587 | 6.622  | 68.088 | 1.00 | 55.67 |
| ATOM | 2556 | CD2 | LEU | B | 44 | 36.446 | 5.433  | 69.276 | 1.00 | 48.14 |
| ATOM | 2557 | C   | LEU | B | 44 | 37.551 | 3.568  | 66.793 | 1.00 | 59.86 |
| ATOM | 2558 | O   | LEU | B | 44 | 38.446 | 4.143  | 66.175 | 1.00 | 48.99 |
| ATOM | 2559 | N   | SER | B | 45 | 37.750 | 2.840  | 67.887 | 1.00 | 64.48 |
| ATOM | 2560 | CA  | SER | B | 45 | 39.072 | 2.646  | 68.456 | 1.00 | 71.61 |
| ATOM | 2561 | CB  | SER | B | 45 | 39.047 | 1.584  | 69.560 | 1.00 | 73.68 |
| ATOM | 2562 | OG  | SER | B | 45 | 40.284 | 0.883  | 69.574 | 1.00 | 76.78 |
| ATOM | 2563 | C   | SER | B | 45 | 40.089 | 2.224  | 67.396 | 1.00 | 71.36 |
| ATOM | 2564 | O   | SER | B | 45 | 41.209 | 2.728  | 67.377 | 1.00 | 52.39 |
| ATOM | 2565 | N   | LYS | B | 46 | 39.662 | 1.295  | 66.549 | 1.00 | 78.57 |
| ATOM | 2566 | CA  | LYS | B | 46 | 40.501 | 0.742  | 65.494 | 1.00 | 84.31 |
| ATOM | 2567 | CB  | LYS | B | 46 | 39.848 | -0.499 | 64.885 | 1.00 | 89.10 |
| ATOM | 2568 | CG  | LYS | B | 46 | 40.772 | -1.693 | 64.707 | 1.00 | 85.70 |
| ATOM | 2569 | CD  | LYS | B | 46 | 40.699 | -2.236 | 63.288 | 1.00 | 83.59 |
| ATOM | 2570 | CE  | LYS | B | 46 | 41.199 | -3.666 | 63.201 | 1.00 | 84.74 |
| ATOM | 2571 | NZ  | LYS | B | 46 | 40.192 | -4.641 | 63.706 | 1.00 | 92.84 |
| ATOM | 2572 | C   | LYS | B | 46 | 40.773 | 1.795  | 64.420 | 1.00 | 81.13 |
| ATOM | 2573 | O   | LYS | B | 46 | 41.920 | 1.966  | 64.005 | 1.00 | 84.85 |
| ATOM | 2574 | N   | GLU | B | 47 | 39.718 | 2.485  | 64.012 | 1.00 | 74.35 |
| ATOM | 2575 | CA  | GLU | B | 47 | 39.755 | 3.570  | 63.041 | 1.00 | 70.19 |
| ATOM | 2576 | CB  | GLU | B | 47 | 38.323 | 3.963  | 62.661 | 1.00 | 66.52 |
| ATOM | 2577 | CG  | GLU | B | 47 | 38.025 | 5.446  | 62.668 | 1.00 | 62.55 |
| ATOM | 2578 | CD  | GLU | B | 47 | 36.885 | 5.861  | 61.763 | 1.00 | 59.88 |
| ATOM | 2579 | OE1 | GLU | B | 47 | 36.350 | 5.017  | 61.015 | 1.00 | 48.61 |
| ATOM | 2580 | OE2 | GLU | B | 47 | 36.514 | 7.057  | 61.794 | 1.00 | 47.49 |
| ATOM | 2581 | C   | GLU | B | 47 | 40.536 | 4.777  | 63.555 | 1.00 | 65.98 |
| ATOM | 2582 | O   | GLU | B | 47 | 40.806 | 5.729  | 62.818 | 1.00 | 61.94 |
| ATOM | 2583 | N   | TYR | B | 48 | 40.929 | 4.759  | 64.822 | 1.00 | 59.02 |
| ATOM | 2584 | CA  | TYR | B | 48 | 41.740 | 5.813  | 65.412 | 1.00 | 54.32 |
| ATOM | 2585 | CB  | TYR | B | 48 | 41.164 | 6.221  | 66.766 | 1.00 | 47.04 |
| ATOM | 2586 | CG  | TYR | B | 48 | 41.966 | 7.305  | 67.448 | 1.00 | 43.40 |
| ATOM | 2587 | CD1 | TYR | B | 48 | 41.837 | 8.629  | 67.048 | 1.00 | 39.64 |
| ATOM | 2588 | CE1 | TYR | B | 48 | 42.565 | 9.622  | 67.667 | 1.00 | 35.48 |
| ATOM | 2589 | CZ  | TYR | B | 48 | 43.426 | 9.313  | 68.688 | 1.00 | 33.02 |
| ATOM | 2590 | OH  | TYR | B | 48 | 44.149 | 10.314 | 69.302 | 1.00 | 49.28 |
| ATOM | 2591 | CE2 | TYR | B | 48 | 43.570 | 8.007  | 69.103 | 1.00 | 43.77 |
| ATOM | 2592 | CD2 | TYR | B | 48 | 42.842 | 7.011  | 68.481 | 1.00 | 38.80 |
| ATOM | 2593 | C   | TYR | B | 48 | 43.182 | 5.374  | 65.585 | 1.00 | 59.37 |
| ATOM | 2594 | O   | TYR | B | 48 | 44.124 | 6.169  | 65.563 | 1.00 | 53.93 |
| ATOM | 2595 | N   | GLU | B | 49 | 43.427 | 4.067  | 65.759 | 1.00 | 56.83 |
| ATOM | 2596 | CA  | GLU | B | 49 | 44.857 | 3.719  | 65.788 | 1.00 | 52.72 |
| ATOM | 2597 | CB  | GLU | B | 49 | 45.118 | 2.439  | 66.568 | 1.00 | 61.99 |
| ATOM | 2598 | CG  | GLU | B | 49 | 46.098 | 2.586  | 67.723 | 1.00 | 66.59 |
| ATOM | 2599 | CD  | GLU | B | 49 | 45.724 | 3.661  | 68.723 | 1.00 | 68.99 |

**FIGURE 152**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2600 | OE1 | GLU | B | 49 | 44.737 | 3.486  | 69.468 | 1.00 | 71.09 |
| ATOM | 2601 | OE2 | GLU | B | 49 | 46.424 | 4.699  | 68.778 | 1.00 | 64.67 |
| ATOM | 2602 | C   | GLU | B | 49 | 45.353 | 3.635  | 64.349 | 1.00 | 43.12 |
| ATOM | 2603 | O   | GLU | B | 49 | 46.539 | 3.492  | 64.069 | 1.00 | 46.58 |
| ATOM | 2604 | N   | GLU | B | 50 | 44.424 | 3.733  | 63.404 | 1.00 | 35.51 |
| ATOM | 2605 | CA  | GLU | B | 50 | 44.790 | 3.731  | 61.992 | 1.00 | 48.92 |
| ATOM | 2606 | CB  | GLU | B | 50 | 43.546 | 3.509  | 61.132 | 1.00 | 55.98 |
| ATOM | 2607 | CG  | GLU | B | 50 | 43.820 | 2.894  | 59.769 | 1.00 | 62.45 |
| ATOM | 2608 | CD  | GLU | B | 50 | 42.672 | 3.111  | 58.802 | 1.00 | 72.64 |
| ATOM | 2609 | OE1 | GLU | B | 50 | 42.932 | 3.465  | 57.632 | 1.00 | 97.10 |
| ATOM | 2610 | OE2 | GLU | B | 50 | 41.505 | 2.932  | 59.214 | 1.00 | 90.89 |
| ATOM | 2611 | C   | GLU | B | 50 | 45.484 | 5.036  | 61.609 | 1.00 | 51.81 |
| ATOM | 2612 | O   | GLU | B | 50 | 46.447 | 5.031  | 60.840 | 1.00 | 60.14 |
| ATOM | 2613 | N   | LEU | B | 51 | 44.993 | 6.142  | 62.157 | 1.00 | 45.17 |
| ATOM | 2614 | CA  | LEU | B | 51 | 45.544 | 7.474  | 61.921 | 1.00 | 36.37 |
| ATOM | 2615 | CB  | LEU | B | 51 | 44.599 | 8.527  | 62.511 | 1.00 | 31.85 |
| ATOM | 2616 | CG  | LEU | B | 51 | 43.381 | 8.867  | 61.656 | 1.00 | 28.95 |
| ATOM | 2617 | CD1 | LEU | B | 51 | 42.269 | 9.488  | 62.490 | 1.00 | 29.93 |
| ATOM | 2618 | CD2 | LEU | B | 51 | 43.770 | 9.789  | 60.507 | 1.00 | 38.39 |
| ATOM | 2619 | C   | LEU | B | 51 | 46.931 | 7.623  | 62.529 | 1.00 | 40.25 |
| ATOM | 2620 | O   | LEU | B | 51 | 47.666 | 8.567  | 62.254 | 1.00 | 43.39 |
| ATOM | 2621 | N   | LYS | B | 52 | 47.288 | 6.661  | 63.367 | 1.00 | 39.11 |
| ATOM | 2622 | CA  | LYS | B | 52 | 48.486 | 6.628  | 64.172 | 1.00 | 41.30 |
| ATOM | 2623 | CB  | LYS | B | 52 | 48.607 | 5.228  | 64.795 | 1.00 | 38.29 |
| ATOM | 2624 | CG  | LYS | B | 52 | 49.077 | 5.211  | 66.234 | 1.00 | 41.48 |
| ATOM | 2625 | CD  | LYS | B | 52 | 49.745 | 3.871  | 66.543 | 1.00 | 42.51 |
| ATOM | 2626 | CE  | LYS | B | 52 | 49.996 | 3.752  | 68.036 | 1.00 | 44.45 |
| ATOM | 2627 | NZ  | LYS | B | 52 | 48.720 | 3.710  | 68.803 | 1.00 | 54.34 |
| ATOM | 2628 | C   | LYS | B | 52 | 49.776 | 6.939  | 63.433 | 1.00 | 43.04 |
| ATOM | 2629 | O   | LYS | B | 52 | 50.637 | 7.651  | 63.963 | 1.00 | 51.42 |
| ATOM | 2630 | N   | ASP | B | 53 | 49.981 | 6.421  | 62.225 | 1.00 | 35.92 |
| ATOM | 2631 | CA  | ASP | B | 53 | 51.272 | 6.646  | 61.580 | 1.00 | 36.34 |
| ATOM | 2632 | CB  | ASP | B | 53 | 51.714 | 5.388  | 60.823 | 1.00 | 46.86 |
| ATOM | 2633 | CG  | ASP | B | 53 | 51.520 | 4.136  | 61.665 | 1.00 | 60.28 |
| ATOM | 2634 | OD1 | ASP | B | 53 | 50.750 | 3.258  | 61.221 | 1.00 | 74.44 |
| ATOM | 2635 | OD2 | ASP | B | 53 | 52.132 | 4.051  | 62.753 | 1.00 | 57.58 |
| ATOM | 2636 | C   | ASP | B | 53 | 51.267 | 7.819  | 60.606 | 1.00 | 25.54 |
| ATOM | 2637 | O   | ASP | B | 53 | 52.315 | 8.092  | 60.019 | 1.00 | 31.31 |
| ATOM | 2638 | N   | VAL | B | 54 | 50.126 | 8.459  | 60.444 | 1.00 | 25.37 |
| ATOM | 2639 | CA  | VAL | B | 54 | 50.004 | 9.549  | 59.477 | 1.00 | 28.87 |
| ATOM | 2640 | CB  | VAL | B | 54 | 48.603 | 10.168 | 59.522 | 1.00 | 32.29 |
| ATOM | 2641 | CG1 | VAL | B | 54 | 48.397 | 11.175 | 58.399 | 1.00 | 27.43 |
| ATOM | 2642 | CG2 | VAL | B | 54 | 47.541 | 9.073  | 59.433 | 1.00 | 35.45 |
| ATOM | 2643 | C   | VAL | B | 54 | 51.089 | 10.587 | 59.747 | 1.00 | 35.40 |
| ATOM | 2644 | O   | VAL | B | 54 | 51.266 | 11.007 | 60.887 | 1.00 | 28.36 |
| ATOM | 2645 | N   | GLY | B | 55 | 51.818 | 10.950 | 58.704 | 1.00 | 30.35 |
| ATOM | 2646 | CA  | GLY | B | 55 | 52.888 | 11.904 | 58.678 | 1.00 | 26.77 |
| ATOM | 2647 | C   | GLY | B | 55 | 54.129 | 11.566 | 59.459 | 1.00 | 31.10 |
| ATOM | 2648 | O   | GLY | B | 55 | 54.988 | 12.440 | 59.618 | 1.00 | 28.63 |
| ATOM | 2649 | N   | ARG | B | 56 | 54.281 | 10.344 | 59.959 | 1.00 | 31.74 |
| ATOM | 2650 | CA  | ARG | B | 56 | 55.404 | 9.997  | 60.827 | 1.00 | 37.30 |
| ATOM | 2651 | CB  | ARG | B | 56 | 55.077 | 8.697  | 61.573 | 1.00 | 46.87 |

**FIGURE 153**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2652 | CG  | ARG | B | 56 | 55.107 | 7.449  | 60.705 | 1.00 | 56.15 |
| ATOM | 2653 | CD  | ARG | B | 56 | 55.129 | 6.169  | 61.530 | 1.00 | 51.35 |
| ATOM | 2654 | NE  | ARG | B | 56 | 56.387 | 5.999  | 62.253 | 1.00 | 46.32 |
| ATOM | 2655 | CZ  | ARG | B | 56 | 56.583 | 5.142  | 63.245 | 1.00 | 43.24 |
| ATOM | 2656 | NH1 | ARG | B | 56 | 55.595 | 4.357  | 63.646 | 1.00 | 38.49 |
| ATOM | 2657 | NH2 | ARG | B | 56 | 57.771 | 5.074  | 63.831 | 1.00 | 37.94 |
| ATOM | 2658 | C   | ARG | B | 56 | 56.729 | 9.869  | 60.089 | 1.00 | 44.81 |
| ATOM | 2659 | O   | ARG | B | 56 | 57.782 | 9.586  | 60.675 | 1.00 | 33.22 |
| ATOM | 2660 | N   | ASN | B | 57 | 56.702 | 10.084 | 58.779 | 1.00 | 40.44 |
| ATOM | 2661 | CA  | ASN | B | 57 | 57.876 | 10.023 | 57.931 | 1.00 | 33.30 |
| ATOM | 2662 | CB  | ASN | B | 57 | 57.436 | 9.773  | 56.482 | 1.00 | 44.90 |
| ATOM | 2663 | CG  | ASN | B | 57 | 56.483 | 10.848 | 55.987 | 1.00 | 53.38 |
| ATOM | 2664 | OD1 | ASN | B | 57 | 56.798 | 11.576 | 55.040 | 1.00 | 73.52 |
| ATOM | 2665 | ND2 | ASN | B | 57 | 55.311 | 10.971 | 56.602 | 1.00 | 38.90 |
| ATOM | 2666 | C   | ASN | B | 57 | 58.691 | 11.308 | 57.972 | 1.00 | 31.80 |
| ATOM | 2667 | O   | ASN | B | 57 | 59.810 | 11.344 | 57.465 | 1.00 | 31.72 |
| ATOM | 2668 | N   | GLN | B | 58 | 58.129 | 12.357 | 58.569 | 1.00 | 28.77 |
| ATOM | 2669 | CA  | GLN | B | 58 | 58.736 | 13.681 | 58.549 | 1.00 | 24.41 |
| ATOM | 2670 | CB  | GLN | B | 58 | 57.611 | 14.729 | 58.466 | 1.00 | 27.17 |
| ATOM | 2671 | CG  | GLN | B | 58 | 56.688 | 14.411 | 57.292 | 1.00 | 28.52 |
| ATOM | 2672 | CD  | GLN | B | 58 | 55.494 | 15.335 | 57.233 | 1.00 | 31.70 |
| ATOM | 2673 | OE1 | GLN | B | 58 | 55.513 | 16.340 | 56.520 | 1.00 | 30.23 |
| ATOM | 2674 | NE2 | GLN | B | 58 | 54.460 | 14.991 | 57.992 | 1.00 | 28.20 |
| ATOM | 2675 | C   | GLN | B | 58 | 59.621 | 13.965 | 59.743 | 1.00 | 26.40 |
| ATOM | 2676 | O   | GLN | B | 58 | 59.307 | 13.588 | 60.865 | 1.00 | 32.07 |
| ATOM | 2677 | N   | SER | B | 59 | 60.750 | 14.633 | 59.494 | 1.00 | 21.54 |
| ATOM | 2678 | CA  | SER | B | 59 | 61.713 | 14.878 | 60.552 | 1.00 | 25.17 |
| ATOM | 2679 | CB  | SER | B | 59 | 63.136 | 14.784 | 60.000 | 1.00 | 31.63 |
| ATOM | 2680 | OG  | SER | B | 59 | 63.435 | 15.925 | 59.212 | 1.00 | 43.09 |
| ATOM | 2681 | C   | SER | B | 59 | 61.470 | 16.250 | 61.193 | 1.00 | 29.30 |
| ATOM | 2682 | O   | SER | B | 59 | 60.674 | 17.010 | 60.635 | 1.00 | 24.20 |
| ATOM | 2683 | N   | CYS | B | 60 | 62.166 | 16.479 | 62.290 | 1.00 | 25.59 |
| ATOM | 2684 | CA  | CYS | B | 60 | 62.116 | 17.647 | 63.149 | 1.00 | 30.08 |
| ATOM | 2685 | CB  | CYS | B | 60 | 61.390 | 17.257 | 64.451 | 1.00 | 26.43 |
| ATOM | 2686 | SG  | CYS | B | 60 | 59.647 | 16.884 | 64.130 | 1.00 | 33.04 |
| ATOM | 2687 | C   | CYS | B | 60 | 63.489 | 18.201 | 63.472 | 1.00 | 33.64 |
| ATOM | 2688 | O   | CYS | B | 60 | 63.790 | 18.632 | 64.592 | 1.00 | 25.31 |
| ATOM | 2689 | N   | ASP | B | 61 | 64.361 | 18.193 | 62.463 | 1.00 | 23.90 |
| ATOM | 2690 | CA  | ASP | B | 61 | 65.744 | 18.559 | 62.696 | 1.00 | 19.83 |
| ATOM | 2691 | CB  | ASP | B | 61 | 66.538 | 18.374 | 61.392 | 1.00 | 28.21 |
| ATOM | 2692 | CG  | ASP | B | 61 | 66.602 | 16.912 | 60.974 | 1.00 | 37.45 |
| ATOM | 2693 | OD1 | ASP | B | 61 | 66.668 | 16.033 | 61.857 | 1.00 | 46.92 |
| ATOM | 2694 | OD2 | ASP | B | 61 | 66.585 | 16.633 | 59.756 | 1.00 | 39.28 |
| ATOM | 2695 | C   | ASP | B | 61 | 65.931 | 19.978 | 63.202 | 1.00 | 18.89 |
| ATOM | 2696 | O   | ASP | B | 61 | 66.742 | 20.234 | 64.100 | 1.00 | 26.23 |
| ATOM | 2697 | N   | ILE | B | 62 | 65.208 | 20.944 | 62.642 | 1.00 | 17.76 |
| ATOM | 2698 | CA  | ILE | B | 62 | 65.463 | 22.312 | 63.098 | 1.00 | 16.77 |
| ATOM | 2699 | CB  | ILE | B | 62 | 64.737 | 23.351 | 62.222 | 1.00 | 26.79 |
| ATOM | 2700 | CG1 | ILE | B | 62 | 65.028 | 23.219 | 60.729 | 1.00 | 30.78 |
| ATOM | 2701 | CD1 | ILE | B | 62 | 66.350 | 22.561 | 60.400 | 1.00 | 49.88 |
| ATOM | 2702 | CG2 | ILE | B | 62 | 65.029 | 24.761 | 62.731 | 1.00 | 20.53 |
| ATOM | 2703 | C   | ILE | B | 62 | 65.015 | 22.503 | 64.540 | 1.00 | 21.81 |

**FIGURE 154**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2704 | O   | ILE | B | 62 | 65.635 | 23.218 | 65.328 | 1.00 | 26.45 |
| ATOM | 2705 | N   | ALA | B | 63 | 63.903 | 21.860 | 64.890 | 1.00 | 22.22 |
| ATOM | 2706 | CA  | ALA | B | 63 | 63.421 | 22.042 | 66.267 | 1.00 | 23.49 |
| ATOM | 2707 | CB  | ALA | B | 63 | 62.039 | 21.427 | 66.404 | 1.00 | 13.73 |
| ATOM | 2708 | C   | ALA | B | 63 | 64.438 | 21.456 | 67.235 | 1.00 | 32.72 |
| ATOM | 2709 | O   | ALA | B | 63 | 64.621 | 21.898 | 68.366 | 1.00 | 29.49 |
| ATOM | 2710 | N   | LEU | B | 64 | 65.142 | 20.427 | 66.770 | 1.00 | 26.75 |
| ATOM | 2711 | CA  | LEU | B | 64 | 66.097 | 19.704 | 67.590 | 1.00 | 24.87 |
| ATOM | 2712 | CB  | LEU | B | 64 | 66.248 | 18.272 | 67.035 | 1.00 | 30.01 |
| ATOM | 2713 | CG  | LEU | B | 64 | 65.032 | 17.393 | 67.356 | 1.00 | 30.13 |
| ATOM | 2714 | CD1 | LEU | B | 64 | 65.068 | 16.082 | 66.591 | 1.00 | 23.61 |
| ATOM | 2715 | CD2 | LEU | B | 64 | 64.982 | 17.171 | 68.862 | 1.00 | 35.44 |
| ATOM | 2716 | C   | LEU | B | 64 | 67.454 | 20.371 | 67.657 | 1.00 | 28.99 |
| ATOM | 2717 | O   | LEU | B | 64 | 68.343 | 19.889 | 68.367 | 1.00 | 41.07 |
| ATOM | 2718 | N   | LEU | B | 65 | 67.636 | 21.470 | 66.927 | 1.00 | 26.97 |
| ATOM | 2719 | CA  | LEU | B | 65 | 68.925 | 22.152 | 66.964 | 1.00 | 25.83 |
| ATOM | 2720 | CB  | LEU | B | 65 | 68.955 | 23.340 | 66.001 | 1.00 | 29.04 |
| ATOM | 2721 | CG  | LEU | B | 65 | 69.017 | 23.002 | 64.513 | 1.00 | 33.55 |
| ATOM | 2722 | CD1 | LEU | B | 65 | 68.843 | 24.264 | 63.679 | 1.00 | 36.14 |
| ATOM | 2723 | CD2 | LEU | B | 65 | 70.327 | 22.301 | 64.180 | 1.00 | 39.25 |
| ATOM | 2724 | C   | LEU | B | 65 | 69.234 | 22.654 | 68.373 | 1.00 | 30.40 |
| ATOM | 2725 | O   | LEU | B | 65 | 68.329 | 23.174 | 69.021 | 1.00 | 31.08 |
| ATOM | 2726 | N   | PRO | B | 66 | 70.470 | 22.487 | 68.809 | 1.00 | 33.09 |
| ATOM | 2727 | CA  | PRO | B | 66 | 70.935 | 22.972 | 70.112 | 1.00 | 41.49 |
| ATOM | 2728 | CB  | PRO | B | 66 | 72.456 | 23.052 | 69.889 | 1.00 | 43.28 |
| ATOM | 2729 | CG  | PRO | B | 66 | 72.722 | 21.860 | 69.020 | 1.00 | 38.43 |
| ATOM | 2730 | CD  | PRO | B | 66 | 71.543 | 21.766 | 68.091 | 1.00 | 35.99 |
| ATOM | 2731 | C   | PRO | B | 66 | 70.390 | 24.336 | 70.511 | 1.00 | 44.08 |
| ATOM | 2732 | O   | PRO | B | 66 | 69.735 | 24.440 | 71.557 | 1.00 | 50.98 |
| ATOM | 2733 | N   | GLU | B | 67 | 70.636 | 25.375 | 69.722 | 1.00 | 35.08 |
| ATOM | 2734 | CA  | GLU | B | 67 | 70.246 | 26.724 | 70.105 | 1.00 | 39.35 |
| ATOM | 2735 | CB  | GLU | B | 67 | 70.775 | 27.730 | 69.068 | 1.00 | 38.98 |
| ATOM | 2736 | CG  | GLU | B | 67 | 71.059 | 27.062 | 67.732 | 1.00 | 52.87 |
| ATOM | 2737 | CD  | GLU | B | 67 | 70.712 | 27.954 | 66.555 | 1.00 | 59.99 |
| ATOM | 2738 | OE1 | GLU | B | 67 | 71.040 | 29.158 | 66.611 | 1.00 | 78.27 |
| ATOM | 2739 | OE2 | GLU | B | 67 | 70.119 | 27.433 | 65.586 | 1.00 | 46.11 |
| ATOM | 2740 | C   | GLU | B | 67 | 68.744 | 26.916 | 70.246 | 1.00 | 38.16 |
| ATOM | 2741 | O   | GLU | B | 67 | 68.327 | 27.971 | 70.736 | 1.00 | 36.75 |
| ATOM | 2742 | N   | ASN | B | 68 | 67.935 | 25.950 | 69.821 | 1.00 | 29.98 |
| ATOM | 2743 | CA  | ASN | B | 68 | 66.493 | 26.069 | 69.927 | 1.00 | 24.34 |
| ATOM | 2744 | CB  | ASN | B | 68 | 65.775 | 25.589 | 68.662 | 1.00 | 22.49 |
| ATOM | 2745 | CG  | ASN | B | 68 | 66.037 | 26.469 | 67.459 | 1.00 | 23.36 |
| ATOM | 2746 | OD1 | ASN | B | 68 | 66.205 | 27.674 | 67.613 | 1.00 | 24.40 |
| ATOM | 2747 | ND2 | ASN | B | 68 | 66.092 | 25.871 | 66.273 | 1.00 | 19.47 |
| ATOM | 2748 | C   | ASN | B | 68 | 65.957 | 25.255 | 71.100 | 1.00 | 28.35 |
| ATOM | 2749 | O   | ASN | B | 68 | 64.733 | 25.161 | 71.233 | 1.00 | 31.84 |
| ATOM | 2750 | N   | ARG | B | 69 | 66.821 | 24.667 | 71.924 | 1.00 | 28.07 |
| ATOM | 2751 | CA  | ARG | B | 69 | 66.284 | 23.759 | 72.950 | 1.00 | 39.17 |
| ATOM | 2752 | CB  | ARG | B | 69 | 67.429 | 23.142 | 73.757 | 1.00 | 53.87 |
| ATOM | 2753 | CG  | ARG | B | 69 | 66.997 | 22.065 | 74.739 | 1.00 | 67.65 |
| ATOM | 2754 | CD  | ARG | B | 69 | 68.095 | 21.761 | 75.748 | 1.00 | 84.00 |
| ATOM | 2755 | NE  | ARG | B | 69 | 67.751 | 22.204 | 77.096 | 1.00 | 97.13 |

**FIGURE 155**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |            |
|------|------|-----|-----|---|----|--------|--------|--------|------------|
| ATOM | 2756 | CZ  | ARG | B | 69 | 68.057 | 21.573 | 78.220 | 1.00102.06 |
| ATOM | 2757 | NH1 | ARG | B | 69 | 68.733 | 20.432 | 78.192 | 1.00107.87 |
| ATOM | 2758 | NH2 | ARG | B | 69 | 67.686 | 22.083 | 79.390 | 1.00 97.89 |
| ATOM | 2759 | C   | ARG | B | 69 | 65.290 | 24.445 | 73.877 | 1.00 34.20 |
| ATOM | 2760 | O   | ARG | B | 69 | 64.217 | 23.908 | 74.184 | 1.00 35.41 |
| ATOM | 2761 | N   | GLY | B | 70 | 65.616 | 25.659 | 74.328 | 1.00 21.83 |
| ATOM | 2762 | CA  | GLY | B | 70 | 64.720 | 26.300 | 75.284 | 1.00 24.46 |
| ATOM | 2763 | C   | GLY | B | 70 | 63.455 | 26.843 | 74.655 | 1.00 27.71 |
| ATOM | 2764 | O   | GLY | B | 70 | 62.569 | 27.348 | 75.354 | 1.00 27.30 |
| ATOM | 2765 | N   | LYS | B | 71 | 63.327 | 26.770 | 73.329 | 1.00 24.69 |
| ATOM | 2766 | CA  | LYS | B | 71 | 62.166 | 27.353 | 72.655 | 1.00 22.38 |
| ATOM | 2767 | CB  | LYS | B | 71 | 62.587 | 27.893 | 71.274 | 1.00 24.49 |
| ATOM | 2768 | CG  | LYS | B | 71 | 63.764 | 28.870 | 71.323 | 1.00 19.45 |
| ATOM | 2769 | CD  | LYS | B | 71 | 64.184 | 29.275 | 69.921 | 1.00 23.88 |
| ATOM | 2770 | CE  | LYS | B | 71 | 65.345 | 30.261 | 69.951 | 1.00 28.97 |
| ATOM | 2771 | NZ  | LYS | B | 71 | 66.081 | 30.241 | 68.653 | 1.00 31.46 |
| ATOM | 2772 | C   | LYS | B | 71 | 61.010 | 26.379 | 72.521 | 1.00 17.66 |
| ATOM | 2773 | O   | LYS | B | 71 | 59.934 | 26.726 | 72.014 | 1.00 18.84 |
| ATOM | 2774 | N   | ASN | B | 72 | 61.211 | 25.140 | 72.984 | 1.00 15.08 |
| ATOM | 2775 | CA  | ASN | B | 72 | 60.162 | 24.136 | 72.990 | 1.00 14.64 |
| ATOM | 2776 | CB  | ASN | B | 72 | 60.706 | 22.823 | 72.400 | 1.00 18.63 |
| ATOM | 2777 | CG  | ASN | B | 72 | 61.196 | 23.022 | 70.977 | 1.00 21.72 |
| ATOM | 2778 | OD1 | ASN | B | 72 | 60.464 | 23.572 | 70.157 | 1.00 19.84 |
| ATOM | 2779 | ND2 | ASN | B | 72 | 62.409 | 22.607 | 70.663 | 1.00 16.01 |
| ATOM | 2780 | C   | ASN | B | 72 | 59.640 | 23.891 | 74.408 | 1.00 14.08 |
| ATOM | 2781 | O   | ASN | B | 72 | 60.429 | 23.667 | 75.324 | 1.00 19.73 |
| ATOM | 2782 | N   | ARG | B | 73 | 58.334 | 23.951 | 74.601 | 1.00 15.40 |
| ATOM | 2783 | CA  | ARG | B | 73 | 57.720 | 23.714 | 75.893 | 1.00 23.30 |
| ATOM | 2784 | CB  | ARG | B | 73 | 56.221 | 23.993 | 75.832 | 1.00 17.66 |
| ATOM | 2785 | CG  | ARG | B | 73 | 55.551 | 23.888 | 77.187 | 1.00 14.92 |
| ATOM | 2786 | CD  | ARG | B | 73 | 54.140 | 24.412 | 77.108 | 1.00 14.81 |
| ATOM | 2787 | NE  | ARG | B | 73 | 54.131 | 25.882 | 77.110 | 1.00 17.20 |
| ATOM | 2788 | CZ  | ARG | B | 73 | 54.259 | 26.568 | 78.241 | 1.00 22.34 |
| ATOM | 2789 | NH1 | ARG | B | 73 | 54.403 | 25.967 | 79.421 | 1.00 13.10 |
| ATOM | 2790 | NH2 | ARG | B | 73 | 54.229 | 27.883 | 78.127 | 1.00 19.63 |
| ATOM | 2791 | C   | ARG | B | 73 | 57.917 | 22.253 | 76.319 | 1.00 28.40 |
| ATOM | 2792 | O   | ARG | B | 73 | 58.144 | 21.962 | 77.484 | 1.00 19.38 |
| ATOM | 2793 | N   | TYR | B | 74 | 57.810 | 21.373 | 75.335 | 1.00 22.53 |
| ATOM | 2794 | CA  | TYR | B | 74 | 57.930 | 19.925 | 75.513 | 1.00 16.28 |
| ATOM | 2795 | CB  | TYR | B | 74 | 56.580 | 19.271 | 75.323 | 1.00 19.24 |
| ATOM | 2796 | CG  | TYR | B | 74 | 55.438 | 19.771 | 76.176 | 1.00 19.80 |
| ATOM | 2797 | CD1 | TYR | B | 74 | 55.345 | 19.402 | 77.515 | 1.00 21.42 |
| ATOM | 2798 | CE1 | TYR | B | 74 | 54.301 | 19.844 | 78.304 | 1.00 21.50 |
| ATOM | 2799 | CZ  | TYR | B | 74 | 53.324 | 20.663 | 77.785 | 1.00 18.77 |
| ATOM | 2800 | OH  | TYR | B | 74 | 52.288 | 21.098 | 78.587 | 1.00 23.74 |
| ATOM | 2801 | CE2 | TYR | B | 74 | 53.379 | 21.045 | 76.460 | 1.00 12.51 |
| ATOM | 2802 | CD2 | TYR | B | 74 | 54.439 | 20.586 | 75.681 | 1.00 13.12 |
| ATOM | 2803 | C   | TYR | B | 74 | 58.958 | 19.399 | 74.521 | 1.00 22.96 |
| ATOM | 2804 | O   | TYR | B | 74 | 58.901 | 19.662 | 73.319 | 1.00 22.52 |
| ATOM | 2805 | N   | ASN | B | 75 | 59.951 | 18.640 | 74.966 | 1.00 26.45 |
| ATOM | 2806 | CA  | ASN | B | 75 | 61.042 | 18.268 | 74.058 | 1.00 23.82 |
| ATOM | 2807 | CB  | ASN | B | 75 | 62.205 | 17.736 | 74.904 | 1.00 32.86 |

**FIGURE 156**



Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2808 | CG  | ASN | B | 75 | 62.817 | 18.860 | 75.726 | 1.00 | 45.64 |
| ATOM | 2809 | OD1 | ASN | B | 75 | 63.098 | 18.687 | 76.911 | 1.00 | 76.89 |
| ATOM | 2810 | ND2 | ASN | B | 75 | 63.024 | 20.023 | 75.113 | 1.00 | 56.37 |
| ATOM | 2811 | C   | ASN | B | 75 | 60.615 | 17.280 | 72.990 | 1.00 | 17.41 |
| ATOM | 2812 | O   | ASN | B | 75 | 61.316 | 17.091 | 71.993 | 1.00 | 28.78 |
| ATOM | 2813 | N   | ASN | B | 76 | 59.458 | 16.656 | 73.144 | 1.00 | 23.38 |
| ATOM | 2814 | CA  | ASN | B | 76 | 58.985 | 15.644 | 72.207 | 1.00 | 29.72 |
| ATOM | 2815 | CB  | ASN | B | 76 | 58.807 | 14.310 | 72.941 | 1.00 | 30.87 |
| ATOM | 2816 | CG  | ASN | B | 76 | 57.687 | 14.316 | 73.956 | 1.00 | 32.40 |
| ATOM | 2817 | OD1 | ASN | B | 76 | 57.263 | 15.350 | 74.472 | 1.00 | 30.85 |
| ATOM | 2818 | ND2 | ASN | B | 76 | 57.182 | 13.123 | 74.264 | 1.00 | 26.52 |
| ATOM | 2819 | C   | ASN | B | 76 | 57.695 | 16.072 | 71.529 | 1.00 | 27.58 |
| ATOM | 2820 | O   | ASN | B | 76 | 56.906 | 15.286 | 71.002 | 1.00 | 20.64 |
| ATOM | 2821 | N   | ILE | B | 77 | 57.457 | 17.394 | 71.539 | 1.00 | 21.12 |
| ATOM | 2822 | CA  | ILE | B | 77 | 56.355 | 17.899 | 70.728 | 1.00 | 21.78 |
| ATOM | 2823 | CB  | ILE | B | 77 | 55.141 | 18.381 | 71.519 | 1.00 | 18.13 |
| ATOM | 2824 | CG1 | ILE | B | 77 | 54.513 | 17.334 | 72.446 | 1.00 | 20.08 |
| ATOM | 2825 | CD1 | ILE | B | 77 | 53.650 | 16.337 | 71.722 | 1.00 | 23.88 |
| ATOM | 2826 | CG2 | ILE | B | 77 | 54.103 | 18.928 | 70.552 | 1.00 | 17.41 |
| ATOM | 2827 | C   | ILE | B | 77 | 56.919 | 19.048 | 69.880 | 1.00 | 21.40 |
| ATOM | 2828 | O   | ILE | B | 77 | 56.994 | 20.175 | 70.348 | 1.00 | 16.51 |
| ATOM | 2829 | N   | LEU | B | 78 | 57.354 | 18.703 | 68.682 | 1.00 | 17.91 |
| ATOM | 2830 | CA  | LEU | B | 78 | 58.074 | 19.610 | 67.792 | 1.00 | 14.62 |
| ATOM | 2831 | CB  | LEU | B | 78 | 59.558 | 19.235 | 67.683 | 1.00 | 19.22 |
| ATOM | 2832 | CG  | LEU | B | 78 | 60.190 | 18.709 | 68.980 | 1.00 | 24.19 |
| ATOM | 2833 | CD1 | LEU | B | 78 | 61.387 | 17.832 | 68.669 | 1.00 | 25.60 |
| ATOM | 2834 | CD2 | LEU | B | 78 | 60.571 | 19.861 | 69.903 | 1.00 | 24.35 |
| ATOM | 2835 | C   | LEU | B | 78 | 57.435 | 19.608 | 66.409 | 1.00 | 18.54 |
| ATOM | 2836 | O   | LEU | B | 78 | 56.815 | 18.637 | 65.968 | 1.00 | 20.82 |
| ATOM | 2837 | N   | PRO | B | 79 | 57.571 | 20.731 | 65.709 | 1.00 | 20.55 |
| ATOM | 2838 | CA  | PRO | B | 79 | 56.989 | 20.844 | 64.367 | 1.00 | 19.22 |
| ATOM | 2839 | CB  | PRO | B | 79 | 57.039 | 22.345 | 64.119 | 1.00 | 13.66 |
| ATOM | 2840 | CG  | PRO | B | 79 | 58.250 | 22.790 | 64.870 | 1.00 | 15.94 |
| ATOM | 2841 | CD  | PRO | B | 79 | 58.277 | 21.944 | 66.121 | 1.00 | 16.86 |
| ATOM | 2842 | C   | PRO | B | 79 | 57.883 | 20.131 | 63.351 | 1.00 | 11.53 |
| ATOM | 2843 | O   | PRO | B | 79 | 59.095 | 20.108 | 63.519 | 1.00 | 19.21 |
| ATOM | 2844 | N   | TYR | B | 80 | 57.241 | 19.570 | 62.352 | 1.00 | 16.10 |
| ATOM | 2845 | CA  | TYR | B | 80 | 57.888 | 18.998 | 61.189 | 1.00 | 18.42 |
| ATOM | 2846 | CB  | TYR | B | 80 | 56.838 | 18.332 | 60.309 | 1.00 | 19.59 |
| ATOM | 2847 | CG  | TYR | B | 80 | 56.182 | 17.120 | 60.923 | 1.00 | 16.10 |
| ATOM | 2848 | CD1 | TYR | B | 80 | 56.947 | 16.162 | 61.577 | 1.00 | 18.02 |
| ATOM | 2849 | CE1 | TYR | B | 80 | 56.303 | 15.060 | 62.124 | 1.00 | 17.97 |
| ATOM | 2850 | CZ  | TYR | B | 80 | 54.947 | 14.908 | 62.021 | 1.00 | 19.16 |
| ATOM | 2851 | OH  | TYR | B | 80 | 54.319 | 13.807 | 62.575 | 1.00 | 29.70 |
| ATOM | 2852 | CE2 | TYR | B | 80 | 54.174 | 15.848 | 61.375 | 1.00 | 23.11 |
| ATOM | 2853 | CD2 | TYR | B | 80 | 54.816 | 16.945 | 60.831 | 1.00 | 16.60 |
| ATOM | 2854 | C   | TYR | B | 80 | 58.596 | 20.101 | 60.399 | 1.00 | 23.17 |
| ATOM | 2855 | O   | TYR | B | 80 | 58.013 | 21.187 | 60.227 | 1.00 | 20.07 |
| ATOM | 2856 | N   | ASP | B | 81 | 59.813 | 19.801 | 59.961 | 1.00 | 18.92 |
| ATOM | 2857 | CA  | ASP | B | 81 | 60.613 | 20.748 | 59.186 | 1.00 | 25.46 |
| ATOM | 2858 | CB  | ASP | B | 81 | 61.883 | 20.083 | 58.649 | 1.00 | 35.12 |
| ATOM | 2859 | CG  | ASP | B | 81 | 62.912 | 19.827 | 59.726 | 1.00 | 34.96 |

**FIGURE 157**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |       |
|------|------|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 2860 | OD1 | ASP | B | 81 | 62.916 | 20.589 | 60.714 | 1.00 | 26.58 |
| ATOM | 2861 | OD2 | ASP | B | 81 | 63.711 | 18.878 | 59.602 | 1.00 | 34.17 |
| ATOM | 2862 | C   | ASP | B | 81 | 59.815 | 21.292 | 58.006 | 1.00 | 24.68 |
| ATOM | 2863 | O   | ASP | B | 81 | 59.877 | 22.476 | 57.667 | 1.00 | 30.63 |
| ATOM | 2864 | N   | ALA | B | 82 | 59.076 | 20.393 | 57.377 | 1.00 | 21.31 |
| ATOM | 2865 | CA  | ALA | B | 82 | 58.381 | 20.689 | 56.123 | 1.00 | 26.95 |
| ATOM | 2866 | CB  | ALA | B | 82 | 57.912 | 19.386 | 55.477 | 1.00 | 20.31 |
| ATOM | 2867 | C   | ALA | B | 82 | 57.202 | 21.637 | 56.283 | 1.00 | 33.87 |
| ATOM | 2868 | O   | ALA | B | 82 | 56.749 | 22.267 | 55.323 | 1.00 | 20.97 |
| ATOM | 2869 | N   | THR | B | 83 | 56.636 | 21.770 | 57.486 | 1.00 | 28.89 |
| ATOM | 2870 | CA  | THR | B | 83 | 55.445 | 22.602 | 57.616 | 1.00 | 17.68 |
| ATOM | 2871 | CB  | THR | B | 83 | 54.208 | 21.738 | 57.906 | 1.00 | 21.79 |
| ATOM | 2872 | OG1 | THR | B | 83 | 54.406 | 21.013 | 59.135 | 1.00 | 23.91 |
| ATOM | 2873 | CG2 | THR | B | 83 | 54.006 | 20.709 | 56.804 | 1.00 | 19.27 |
| ATOM | 2874 | C   | THR | B | 83 | 55.581 | 23.645 | 58.723 | 1.00 | 17.70 |
| ATOM | 2875 | O   | THR | B | 83 | 54.598 | 24.307 | 59.062 | 1.00 | 19.85 |
| ATOM | 2876 | N   | ARG | B | 84 | 56.768 | 23.799 | 59.299 | 1.00 | 17.15 |
| ATOM | 2877 | CA  | ARG | B | 84 | 56.880 | 24.747 | 60.406 | 1.00 | 21.26 |
| ATOM | 2878 | CB  | ARG | B | 84 | 58.224 | 24.629 | 61.116 | 1.00 | 18.18 |
| ATOM | 2879 | CG  | ARG | B | 84 | 59.419 | 25.008 | 60.264 | 1.00 | 19.29 |
| ATOM | 2880 | CD  | ARG | B | 84 | 60.737 | 24.812 | 60.999 | 1.00 | 26.01 |
| ATOM | 2881 | NE  | ARG | B | 84 | 61.852 | 25.270 | 60.167 | 1.00 | 27.31 |
| ATOM | 2882 | CZ  | ARG | B | 84 | 62.526 | 26.386 | 60.390 | 1.00 | 21.69 |
| ATOM | 2883 | NH1 | ARG | B | 84 | 62.193 | 27.161 | 61.422 | 1.00 | 22.24 |
| ATOM | 2884 | NH2 | ARG | B | 84 | 63.521 | 26.738 | 59.595 | 1.00 | 19.19 |
| ATOM | 2885 | C   | ARG | B | 84 | 56.677 | 26.175 | 59.897 | 1.00 | 24.93 |
| ATOM | 2886 | O   | ARG | B | 84 | 56.868 | 26.452 | 58.713 | 1.00 | 16.17 |
| ATOM | 2887 | N   | VAL | B | 85 | 56.283 | 27.055 | 60.809 | 1.00 | 19.84 |
| ATOM | 2888 | CA  | VAL | B | 85 | 56.219 | 28.487 | 60.544 | 1.00 | 18.69 |
| ATOM | 2889 | CB  | VAL | B | 85 | 55.146 | 29.192 | 61.386 | 1.00 | 16.28 |
| ATOM | 2890 | CG1 | VAL | B | 85 | 55.102 | 30.685 | 61.039 | 1.00 | 23.59 |
| ATOM | 2891 | CG2 | VAL | B | 85 | 53.777 | 28.590 | 61.148 | 1.00 | 12.01 |
| ATOM | 2892 | C   | VAL | B | 85 | 57.571 | 29.131 | 60.815 | 1.00 | 17.55 |
| ATOM | 2893 | O   | VAL | B | 85 | 58.203 | 28.908 | 61.852 | 1.00 | 25.85 |
| ATOM | 2894 | N   | LYS | B | 86 | 58.044 | 29.941 | 59.868 | 1.00 | 18.16 |
| ATOM | 2895 | CA  | LYS | B | 86 | 59.348 | 30.575 | 60.022 | 1.00 | 22.13 |
| ATOM | 2896 | CB  | LYS | B | 86 | 60.149 | 30.469 | 58.717 | 1.00 | 23.96 |
| ATOM | 2897 | CG  | LYS | B | 86 | 60.650 | 29.070 | 58.416 | 1.00 | 23.28 |
| ATOM | 2898 | CD  | LYS | B | 86 | 60.864 | 28.859 | 56.929 | 1.00 | 35.17 |
| ATOM | 2899 | CE  | LYS | B | 86 | 61.343 | 27.446 | 56.630 | 1.00 | 42.63 |
| ATOM | 2900 | NZ  | LYS | B | 86 | 62.795 | 27.284 | 56.931 | 1.00 | 62.83 |
| ATOM | 2901 | C   | LYS | B | 86 | 59.240 | 32.051 | 60.400 | 1.00 | 25.13 |
| ATOM | 2902 | O   | LYS | B | 86 | 58.381 | 32.768 | 59.867 | 1.00 | 22.58 |
| ATOM | 2903 | N   | LEU | B | 87 | 60.112 | 32.497 | 61.294 | 1.00 | 23.50 |
| ATOM | 2904 | CA  | LEU | B | 87 | 60.204 | 33.921 | 61.604 | 1.00 | 27.10 |
| ATOM | 2905 | CB  | LEU | B | 87 | 60.653 | 34.189 | 63.033 | 1.00 | 25.75 |
| ATOM | 2906 | CG  | LEU | B | 87 | 59.927 | 33.453 | 64.164 | 1.00 | 30.29 |
| ATOM | 2907 | CD1 | LEU | B | 87 | 60.620 | 33.695 | 65.499 | 1.00 | 34.70 |
| ATOM | 2908 | CD2 | LEU | B | 87 | 58.467 | 33.866 | 64.258 | 1.00 | 17.70 |
| ATOM | 2909 | C   | LEU | B | 87 | 61.205 | 34.550 | 60.631 | 1.00 | 35.83 |
| ATOM | 2910 | O   | LEU | B | 87 | 62.080 | 33.839 | 60.127 | 1.00 | 31.73 |
| ATOM | 2911 | N   | SER | B | 88 | 61.082 | 35.842 | 60.383 | 1.00 | 37.78 |

**FIGURE 158**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |        |        |      |        |
|------|------|-----|-----|---|----|--------|--------|--------|------|--------|
| ATOM | 2912 | CA  | SER | B | 88 | 62.022 | 36.595 | 59.565 | 1.00 | 39.22  |
| ATOM | 2913 | CB  | SER | B | 88 | 61.501 | 38.024 | 59.360 | 1.00 | 37.70  |
| ATOM | 2914 | OG  | SER | B | 88 | 62.058 | 38.842 | 60.384 | 1.00 | 56.30  |
| ATOM | 2915 | C   | SER | B | 88 | 63.405 | 36.685 | 60.202 | 1.00 | 54.75  |
| ATOM | 2916 | O   | SER | B | 88 | 63.540 | 36.552 | 61.419 | 1.00 | 56.41  |
| ATOM | 2917 | N   | ASN | B | 89 | 64.420 | 36.927 | 59.382 | 1.00 | 75.33  |
| ATOM | 2918 | CA  | ASN | B | 89 | 65.802 | 37.090 | 59.812 | 1.00 | 89.87  |
| ATOM | 2919 | CB  | ASN | B | 89 | 66.720 | 37.253 | 58.599 | 1.00 | 90.11  |
| ATOM | 2920 | CG  | ASN | B | 89 | 66.156 | 38.159 | 57.525 | 1.00 | 90.26  |
| ATOM | 2921 | OD1 | ASN | B | 89 | 65.038 | 38.666 | 57.636 | 1.00 | 84.88  |
| ATOM | 2922 | ND2 | ASN | B | 89 | 66.932 | 38.372 | 56.466 | 1.00 | 89.32  |
| ATOM | 2923 | C   | ASN | B | 89 | 65.966 | 38.281 | 60.749 | 1.00 | 104.61 |
| ATOM | 2924 | O   | ASN | B | 89 | 65.046 | 39.100 | 60.888 | 1.00 | 106.28 |
| ATOM | 2925 | N   | VAL | B | 90 | 67.134 | 38.404 | 61.376 | 1.00 | 117.38 |
| ATOM | 2926 | CA  | VAL | B | 90 | 67.381 | 39.480 | 62.324 | 1.00 | 128.11 |
| ATOM | 2927 | CB  | VAL | B | 90 | 66.614 | 39.227 | 63.643 | 1.00 | 131.44 |
| ATOM | 2928 | CG1 | VAL | B | 90 | 65.182 | 39.743 | 63.544 | 1.00 | 127.66 |
| ATOM | 2929 | CG2 | VAL | B | 90 | 66.623 | 37.744 | 64.000 | 1.00 | 133.27 |
| ATOM | 2930 | C   | VAL | B | 90 | 68.865 | 39.654 | 62.644 | 1.00 | 131.59 |
| ATOM | 2931 | O   | VAL | B | 90 | 69.731 | 39.301 | 61.846 | 1.00 | 124.37 |
| ATOM | 2932 | N   | ASP | B | 91 | 69.146 | 40.207 | 63.826 | 1.00 | 135.31 |
| ATOM | 2933 | CA  | ASP | B | 91 | 70.502 | 40.379 | 64.339 | 1.00 | 137.26 |
| ATOM | 2934 | CB  | ASP | B | 91 | 70.482 | 40.895 | 65.775 | 1.00 | 133.67 |
| ATOM | 2935 | CG  | ASP | B | 91 | 71.529 | 41.944 | 66.104 | 1.00 | 129.34 |
| ATOM | 2936 | OD1 | ASP | B | 91 | 72.177 | 42.475 | 65.180 | 1.00 | 133.28 |
| ATOM | 2937 | OD2 | ASP | B | 91 | 71.709 | 42.256 | 67.303 | 1.00 | 105.69 |
| ATOM | 2938 | C   | ASP | B | 91 | 71.250 | 39.050 | 64.250 | 1.00 | 141.41 |
| ATOM | 2939 | O   | ASP | B | 91 | 70.663 | 38.007 | 64.553 | 1.00 | 146.90 |
| ATOM | 2940 | N   | ASP | B | 92 | 72.513 | 39.087 | 63.838 | 1.00 | 141.54 |
| ATOM | 2941 | CA  | ASP | B | 92 | 73.278 | 37.858 | 63.613 | 1.00 | 138.38 |
| ATOM | 2942 | CB  | ASP | B | 92 | 73.621 | 37.167 | 64.928 | 1.00 | 136.13 |
| ATOM | 2943 | CG  | ASP | B | 92 | 75.034 | 37.428 | 65.408 | 1.00 | 132.67 |
| ATOM | 2944 | OD1 | ASP | B | 92 | 75.913 | 37.722 | 64.570 | 1.00 | 132.34 |
| ATOM | 2945 | OD2 | ASP | B | 92 | 75.280 | 37.340 | 66.632 | 1.00 | 122.69 |
| ATOM | 2946 | C   | ASP | B | 92 | 72.468 | 36.947 | 62.696 | 1.00 | 135.79 |
| ATOM | 2947 | O   | ASP | B | 92 | 71.582 | 37.442 | 61.988 | 1.00 | 127.98 |
| ATOM | 2948 | N   | ASP | B | 93 | 72.728 | 35.641 | 62.690 | 1.00 | 134.71 |
| ATOM | 2949 | CA  | ASP | B | 93 | 71.890 | 34.782 | 61.848 | 1.00 | 133.27 |
| ATOM | 2950 | CB  | ASP | B | 93 | 72.308 | 34.930 | 60.381 | 1.00 | 139.50 |
| ATOM | 2951 | CG  | ASP | B | 93 | 71.490 | 35.955 | 59.623 | 1.00 | 143.40 |
| ATOM | 2952 | OD1 | ASP | B | 93 | 70.243 | 35.893 | 59.679 | 1.00 | 148.49 |
| ATOM | 2953 | OD2 | ASP | B | 93 | 72.087 | 36.837 | 58.963 | 1.00 | 144.76 |
| ATOM | 2954 | C   | ASP | B | 93 | 71.922 | 33.319 | 62.260 | 1.00 | 125.52 |
| ATOM | 2955 | O   | ASP | B | 93 | 72.239 | 32.451 | 61.438 | 1.00 | 114.55 |
| ATOM | 2956 | N   | PRO | B | 94 | 71.590 | 32.989 | 63.500 | 1.00 | 122.86 |
| ATOM | 2957 | CA  | PRO | B | 94 | 71.432 | 31.573 | 63.874 | 1.00 | 118.08 |
| ATOM | 2958 | CB  | PRO | B | 94 | 71.775 | 31.592 | 65.361 | 1.00 | 119.79 |
| ATOM | 2959 | CG  | PRO | B | 94 | 71.314 | 32.928 | 65.833 | 1.00 | 121.96 |
| ATOM | 2960 | CD  | PRO | B | 94 | 71.339 | 33.859 | 64.657 | 1.00 | 123.38 |
| ATOM | 2961 | C   | PRO | B | 94 | 69.991 | 31.145 | 63.644 | 1.00 | 109.34 |
| ATOM | 2962 | O   | PRO | B | 94 | 69.324 | 31.674 | 62.746 | 1.00 | 96.86  |
| ATOM | 2963 | N   | CYS | B | 95 | 69.466 | 30.208 | 64.436 | 1.00 | 101.66 |

**FIGURE 159**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 2964 | CA  | CYS | B | 95  | 68.051 | 29.878 | 64.254 | 1.00 | 88.82  |
| ATOM | 2965 | CB  | CYS | B | 95  | 67.674 | 28.484 | 64.735 | 1.00 | 90.50  |
| ATOM | 2966 | SG  | CYS | B | 95  | 66.393 | 27.656 | 63.760 | 1.00 | 135.13 |
| ATOM | 2967 | C   | CYS | B | 95  | 67.191 | 30.918 | 64.979 | 1.00 | 70.52  |
| ATOM | 2968 | O   | CYS | B | 95  | 66.476 | 30.585 | 65.919 | 1.00 | 43.58  |
| ATOM | 2969 | N   | SER | B | 96  | 67.296 | 32.147 | 64.494 | 1.00 | 60.87  |
| ATOM | 2970 | CA  | SER | B | 96  | 66.446 | 33.248 | 64.919 | 1.00 | 51.63  |
| ATOM | 2971 | CB  | SER | B | 96  | 67.101 | 34.608 | 64.689 | 1.00 | 54.58  |
| ATOM | 2972 | OG  | SER | B | 96  | 67.550 | 34.751 | 63.352 | 1.00 | 59.05  |
| ATOM | 2973 | C   | SER | B | 96  | 65.124 | 33.166 | 64.152 | 1.00 | 37.78  |
| ATOM | 2974 | O   | SER | B | 96  | 64.267 | 34.025 | 64.352 | 1.00 | 49.18  |
| ATOM | 2975 | N   | ASP | B | 97  | 65.021 | 32.137 | 63.309 | 1.00 | 31.64  |
| ATOM | 2976 | CA  | ASP | B | 97  | 63.824 | 31.873 | 62.516 | 1.00 | 27.57  |
| ATOM | 2977 | CB  | ASP | B | 97  | 64.227 | 31.446 | 61.103 | 1.00 | 23.15  |
| ATOM | 2978 | CG  | ASP | B | 97  | 64.442 | 29.970 | 60.866 | 1.00 | 34.09  |
| ATOM | 2979 | OD1 | ASP | B | 97  | 64.645 | 29.151 | 61.783 | 1.00 | 28.80  |
| ATOM | 2980 | OD2 | ASP | B | 97  | 64.413 | 29.585 | 59.675 | 1.00 | 47.02  |
| ATOM | 2981 | C   | ASP | B | 97  | 62.890 | 30.840 | 63.150 | 1.00 | 18.50  |
| ATOM | 2982 | O   | ASP | B | 97  | 61.800 | 30.601 | 62.619 | 1.00 | 19.32  |
| ATOM | 2983 | N   | TYR | B | 98  | 63.315 | 30.229 | 64.254 | 1.00 | 22.52  |
| ATOM | 2984 | CA  | TYR | B | 98  | 62.577 | 29.112 | 64.817 | 1.00 | 19.25  |
| ATOM | 2985 | CB  | TYR | B | 98  | 63.509 | 28.066 | 65.493 | 1.00 | 21.90  |
| ATOM | 2986 | CG  | TYR | B | 98  | 62.669 | 26.947 | 66.087 | 1.00 | 23.21  |
| ATOM | 2987 | CD1 | TYR | B | 98  | 62.108 | 26.015 | 65.211 | 1.00 | 18.81  |
| ATOM | 2988 | CE1 | TYR | B | 98  | 61.328 | 24.979 | 65.683 | 1.00 | 18.20  |
| ATOM | 2989 | CZ  | TYR | B | 98  | 61.098 | 24.872 | 67.048 | 1.00 | 27.42  |
| ATOM | 2990 | OH  | TYR | B | 98  | 60.311 | 23.833 | 67.506 | 1.00 | 16.71  |
| ATOM | 2991 | CE2 | TYR | B | 98  | 61.630 | 25.785 | 67.929 | 1.00 | 16.10  |
| ATOM | 2992 | CD2 | TYR | B | 98  | 62.415 | 26.819 | 67.453 | 1.00 | 15.44  |
| ATOM | 2993 | C   | TYR | B | 98  | 61.524 | 29.537 | 65.833 | 1.00 | 21.92  |
| ATOM | 2994 | O   | TYR | B | 98  | 61.779 | 30.233 | 66.820 | 1.00 | 22.98  |
| ATOM | 2995 | N   | ILE | B | 99  | 60.320 | 29.031 | 65.582 | 1.00 | 16.17  |
| ATOM | 2996 | CA  | ILE | B | 99  | 59.284 | 29.019 | 66.598 | 1.00 | 17.96  |
| ATOM | 2997 | CB  | ILE | B | 99  | 58.282 | 30.173 | 66.466 | 1.00 | 18.22  |
| ATOM | 2998 | CG1 | ILE | B | 99  | 57.208 | 30.134 | 67.564 | 1.00 | 17.54  |
| ATOM | 2999 | CD1 | ILE | B | 99  | 56.327 | 31.368 | 67.580 | 1.00 | 25.26  |
| ATOM | 3000 | CG2 | ILE | B | 99  | 57.629 | 30.221 | 65.094 | 1.00 | 17.90  |
| ATOM | 3001 | C   | ILE | B | 99  | 58.551 | 27.679 | 66.534 | 1.00 | 23.11  |
| ATOM | 3002 | O   | ILE | B | 99  | 58.319 | 27.138 | 65.454 | 1.00 | 19.27  |
| ATOM | 3003 | N   | ASN | B | 100 | 58.185 | 27.139 | 67.694 | 1.00 | 23.62  |
| ATOM | 3004 | CA  | ASN | B | 100 | 57.381 | 25.908 | 67.687 | 1.00 | 17.64  |
| ATOM | 3005 | CB  | ASN | B | 100 | 57.354 | 25.270 | 69.079 | 1.00 | 18.48  |
| ATOM | 3006 | CG  | ASN | B | 100 | 56.794 | 23.863 | 69.078 | 1.00 | 13.37  |
| ATOM | 3007 | OD1 | ASN | B | 100 | 55.775 | 23.626 | 68.446 | 1.00 | 18.56  |
| ATOM | 3008 | ND2 | ASN | B | 100 | 57.453 | 22.935 | 69.780 | 1.00 | 17.03  |
| ATOM | 3009 | C   | ASN | B | 100 | 55.995 | 26.223 | 67.175 | 1.00 | 17.36  |
| ATOM | 3010 | O   | ASN | B | 100 | 55.058 | 26.498 | 67.938 | 1.00 | 16.80  |
| ATOM | 3011 | N   | ALA | B | 101 | 55.867 | 26.172 | 65.839 | 1.00 | 13.82  |
| ATOM | 3012 | CA  | ALA | B | 101 | 54.584 | 26.447 | 65.209 | 1.00 | 8.38   |
| ATOM | 3013 | CB  | ALA | B | 101 | 54.344 | 27.949 | 65.090 | 1.00 | 14.14  |
| ATOM | 3014 | C   | ALA | B | 101 | 54.488 | 25.803 | 63.815 | 1.00 | 10.67  |
| ATOM | 3015 | O   | ALA | B | 101 | 55.532 | 25.598 | 63.187 | 1.00 | 17.26  |

**FIGURE 160**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 3016 | N   | SER B 102 | 53.268 | 25.514 | 63.375 | 1.00 | 10.49 |
| ATOM | 3017 | CA  | SER B 102 | 53.065 | 24.791 | 62.119 | 1.00 | 15.63 |
| ATOM | 3018 | CB  | SER B 102 | 52.782 | 23.308 | 62.372 | 1.00 | 17.37 |
| ATOM | 3019 | OG  | SER B 102 | 53.658 | 22.704 | 63.287 | 1.00 | 15.04 |
| ATOM | 3020 | C   | SER B 102 | 51.879 | 25.328 | 61.337 | 1.00 | 17.17 |
| ATOM | 3021 | O   | SER B 102 | 50.844 | 25.684 | 61.902 | 1.00 | 18.22 |
| ATOM | 3022 | N   | TYR B 103 | 51.990 | 25.368 | 60.011 | 1.00 | 16.28 |
| ATOM | 3023 | CA  | TYR B 103 | 50.851 | 25.708 | 59.172 | 1.00 | 17.81 |
| ATOM | 3024 | CB  | TYR B 103 | 51.321 | 26.133 | 57.778 | 1.00 | 18.72 |
| ATOM | 3025 | CG  | TYR B 103 | 52.139 | 27.398 | 57.701 | 1.00 | 12.87 |
| ATOM | 3026 | CD1 | TYR B 103 | 51.547 | 28.633 | 57.956 | 1.00 | 23.49 |
| ATOM | 3027 | CE1 | TYR B 103 | 52.288 | 29.795 | 57.886 | 1.00 | 21.55 |
| ATOM | 3028 | CZ  | TYR B 103 | 53.619 | 29.769 | 57.564 | 1.00 | 22.19 |
| ATOM | 3029 | OH  | TYR B 103 | 54.334 | 30.948 | 57.499 | 1.00 | 32.87 |
| ATOM | 3030 | CE2 | TYR B 103 | 54.238 | 28.562 | 57.303 | 1.00 | 23.02 |
| ATOM | 3031 | CD2 | TYR B 103 | 53.483 | 27.400 | 57.377 | 1.00 | 19.58 |
| ATOM | 3032 | C   | TYR B 103 | 49.915 | 24.504 | 59.015 | 1.00 | 24.37 |
| ATOM | 3033 | O   | TYR B 103 | 50.388 | 23.378 | 58.803 | 1.00 | 20.89 |
| ATOM | 3034 | N   | ILE B 104 | 48.612 | 24.720 | 59.106 | 1.00 | 17.36 |
| ATOM | 3035 | CA  | ILE B 104 | 47.596 | 23.693 | 58.951 | 1.00 | 20.36 |
| ATOM | 3036 | CB  | ILE B 104 | 46.894 | 23.397 | 60.301 | 1.00 | 24.05 |
| ATOM | 3037 | CG1 | ILE B 104 | 47.859 | 23.206 | 61.472 | 1.00 | 23.04 |
| ATOM | 3038 | CD1 | ILE B 104 | 48.755 | 21.992 | 61.352 | 1.00 | 23.46 |
| ATOM | 3039 | CG2 | ILE B 104 | 45.961 | 22.211 | 60.187 | 1.00 | 28.18 |
| ATOM | 3040 | C   | ILE B 104 | 46.532 | 24.093 | 57.945 | 1.00 | 23.59 |
| ATOM | 3041 | O   | ILE B 104 | 45.944 | 25.175 | 58.016 | 1.00 | 20.30 |
| ATOM | 3042 | N   | PRO B 105 | 46.247 | 23.225 | 56.979 | 1.00 | 20.21 |
| ATOM | 3043 | CA  | PRO B 105 | 45.145 | 23.455 | 56.051 | 1.00 | 17.40 |
| ATOM | 3044 | CB  | PRO B 105 | 45.259 | 22.284 | 55.052 | 1.00 | 20.56 |
| ATOM | 3045 | CG  | PRO B 105 | 46.684 | 21.880 | 55.173 | 1.00 | 22.00 |
| ATOM | 3046 | CD  | PRO B 105 | 46.978 | 21.979 | 56.663 | 1.00 | 22.12 |
| ATOM | 3047 | C   | PRO B 105 | 43.779 | 23.370 | 56.704 | 1.00 | 23.93 |
| ATOM | 3048 | O   | PRO B 105 | 43.584 | 22.625 | 57.664 | 1.00 | 32.98 |
| ATOM | 3049 | N   | GLY B 106 | 42.850 | 24.133 | 56.156 | 1.00 | 21.83 |
| ATOM | 3050 | CA  | GLY B 106 | 41.473 | 24.095 | 56.614 | 1.00 | 27.14 |
| ATOM | 3051 | C   | GLY B 106 | 40.541 | 23.642 | 55.502 | 1.00 | 26.84 |
| ATOM | 3052 | O   | GLY B 106 | 40.994 | 23.136 | 54.472 | 1.00 | 26.33 |
| ATOM | 3053 | N   | ASN B 107 | 39.234 | 23.821 | 55.689 | 1.00 | 23.33 |
| ATOM | 3054 | CA  | ASN B 107 | 38.309 | 23.403 | 54.648 | 1.00 | 33.39 |
| ATOM | 3055 | CB  | ASN B 107 | 36.859 | 23.587 | 55.104 | 1.00 | 40.50 |
| ATOM | 3056 | CG  | ASN B 107 | 36.393 | 22.414 | 55.950 | 1.00 | 42.30 |
| ATOM | 3057 | OD1 | ASN B 107 | 37.022 | 21.357 | 55.975 | 1.00 | 50.74 |
| ATOM | 3058 | ND2 | ASN B 107 | 35.282 | 22.645 | 56.633 | 1.00 | 52.70 |
| ATOM | 3059 | C   | ASN B 107 | 38.485 | 24.195 | 53.354 | 1.00 | 41.23 |
| ATOM | 3060 | O   | ASN B 107 | 38.042 | 23.711 | 52.312 | 1.00 | 34.23 |
| ATOM | 3061 | N   | ASN B 108 | 39.085 | 25.371 | 53.459 | 1.00 | 40.92 |
| ATOM | 3062 | CA  | ASN B 108 | 39.051 | 26.395 | 52.426 | 1.00 | 31.26 |
| ATOM | 3063 | CB  | ASN B 108 | 38.527 | 27.684 | 53.085 | 1.00 | 41.62 |
| ATOM | 3064 | CG  | ASN B 108 | 37.199 | 27.416 | 53.777 | 1.00 | 52.11 |
| ATOM | 3065 | OD1 | ASN B 108 | 36.227 | 27.042 | 53.112 | 1.00 | 34.83 |
| ATOM | 3066 | ND2 | ASN B 108 | 37.163 | 27.598 | 55.094 | 1.00 | 31.17 |
| ATOM | 3067 | C   | ASN B 108 | 40.386 | 26.637 | 51.756 | 1.00 | 31.83 |

**FIGURE 161**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3068 | O   | ASN | B | 108 | 40.482 | 26.772 | 50.534 | 1.00 | 39.22 |
| ATOM | 3069 | N   | PHE | B | 109 | 41.468 | 26.703 | 52.531 | 1.00 | 30.33 |
| ATOM | 3070 | CA  | PHE | B | 109 | 42.774 | 26.919 | 51.911 | 1.00 | 21.96 |
| ATOM | 3071 | CB  | PHE | B | 109 | 43.085 | 28.400 | 51.749 | 1.00 | 20.80 |
| ATOM | 3072 | CG  | PHE | B | 109 | 42.708 | 29.329 | 52.890 | 1.00 | 28.79 |
| ATOM | 3073 | CD1 | PHE | B | 109 | 43.692 | 29.911 | 53.674 | 1.00 | 25.92 |
| ATOM | 3074 | CE1 | PHE | B | 109 | 43.376 | 30.759 | 54.718 | 1.00 | 31.45 |
| ATOM | 3075 | CZ  | PHE | B | 109 | 42.054 | 31.055 | 54.993 | 1.00 | 37.19 |
| ATOM | 3076 | CE2 | PHE | B | 109 | 41.064 | 30.476 | 54.218 | 1.00 | 41.01 |
| ATOM | 3077 | CD2 | PHE | B | 109 | 41.386 | 29.628 | 53.175 | 1.00 | 32.74 |
| ATOM | 3078 | C   | PHE | B | 109 | 43.860 | 26.236 | 52.741 | 1.00 | 20.75 |
| ATOM | 3079 | O   | PHE | B | 109 | 43.593 | 25.834 | 53.871 | 1.00 | 23.61 |
| ATOM | 3080 | N   | ARG | B | 110 | 45.045 | 26.137 | 52.178 | 1.00 | 19.49 |
| ATOM | 3081 | CA  | ARG | B | 110 | 46.176 | 25.416 | 52.710 | 1.00 | 22.84 |
| ATOM | 3082 | CB  | ARG | B | 110 | 47.210 | 25.227 | 51.575 | 1.00 | 21.99 |
| ATOM | 3083 | CG  | ARG | B | 110 | 46.634 | 24.284 | 50.511 | 1.00 | 30.90 |
| ATOM | 3084 | CD  | ARG | B | 110 | 47.726 | 23.349 | 50.019 | 1.00 | 39.83 |
| ATOM | 3085 | NE  | ARG | B | 110 | 47.226 | 22.405 | 49.014 | 1.00 | 54.08 |
| ATOM | 3086 | CZ  | ARG | B | 110 | 47.347 | 21.087 | 49.185 | 1.00 | 72.63 |
| ATOM | 3087 | NH1 | ARG | B | 110 | 47.930 | 20.619 | 50.282 | 1.00 | 79.88 |
| ATOM | 3088 | NH2 | ARG | B | 110 | 46.889 | 20.253 | 48.262 | 1.00 | 87.83 |
| ATOM | 3089 | C   | ARG | B | 110 | 46.863 | 26.073 | 53.890 | 1.00 | 29.52 |
| ATOM | 3090 | O   | ARG | B | 110 | 47.454 | 25.377 | 54.728 | 1.00 | 28.77 |
| ATOM | 3091 | N   | ARG | B | 111 | 46.847 | 27.402 | 53.997 | 1.00 | 20.01 |
| ATOM | 3092 | CA  | ARG | B | 111 | 47.476 | 27.910 | 55.233 | 1.00 | 24.11 |
| ATOM | 3093 | CB  | ARG | B | 111 | 48.635 | 28.837 | 54.943 | 1.00 | 22.68 |
| ATOM | 3094 | CG  | ARG | B | 111 | 49.880 | 28.255 | 54.313 | 1.00 | 19.86 |
| ATOM | 3095 | CD  | ARG | B | 111 | 50.961 | 29.325 | 54.127 | 1.00 | 25.94 |
| ATOM | 3096 | NE  | ARG | B | 111 | 52.272 | 28.701 | 53.923 | 1.00 | 30.60 |
| ATOM | 3097 | CZ  | ARG | B | 111 | 53.449 | 29.295 | 54.017 | 1.00 | 21.38 |
| ATOM | 3098 | NH1 | ARG | B | 111 | 53.524 | 30.583 | 54.324 | 1.00 | 42.58 |
| ATOM | 3099 | NH2 | ARG | B | 111 | 54.570 | 28.620 | 53.808 | 1.00 | 29.00 |
| ATOM | 3100 | C   | ARG | B | 111 | 46.398 | 28.613 | 56.060 | 1.00 | 21.97 |
| ATOM | 3101 | O   | ARG | B | 111 | 46.481 | 29.791 | 56.388 | 1.00 | 19.77 |
| ATOM | 3102 | N   | GLU | B | 112 | 45.354 | 27.865 | 56.383 | 1.00 | 16.17 |
| ATOM | 3103 | CA  | GLU | B | 112 | 44.185 | 28.417 | 57.045 | 1.00 | 16.65 |
| ATOM | 3104 | CB  | GLU | B | 112 | 42.994 | 27.458 | 56.911 | 1.00 | 17.98 |
| ATOM | 3105 | CG  | GLU | B | 112 | 41.678 | 28.188 | 57.126 | 1.00 | 27.35 |
| ATOM | 3106 | CD  | GLU | B | 112 | 40.479 | 27.519 | 56.495 | 1.00 | 27.95 |
| ATOM | 3107 | OE1 | GLU | B | 112 | 39.370 | 27.881 | 56.934 | 1.00 | 28.26 |
| ATOM | 3108 | OE2 | GLU | B | 112 | 40.609 | 26.665 | 55.596 | 1.00 | 25.50 |
| ATOM | 3109 | C   | GLU | B | 112 | 44.461 | 28.700 | 58.518 | 1.00 | 23.99 |
| ATOM | 3110 | O   | GLU | B | 112 | 43.974 | 29.662 | 59.122 | 1.00 | 19.68 |
| ATOM | 3111 | N   | TYR | B | 113 | 45.280 | 27.832 | 59.107 | 1.00 | 19.82 |
| ATOM | 3112 | CA  | TYR | B | 113 | 45.597 | 28.015 | 60.522 | 1.00 | 17.80 |
| ATOM | 3113 | CB  | TYR | B | 113 | 44.940 | 26.997 | 61.450 | 1.00 | 25.68 |
| ATOM | 3114 | CG  | TYR | B | 113 | 43.505 | 26.647 | 61.175 | 1.00 | 20.88 |
| ATOM | 3115 | CD1 | TYR | B | 113 | 43.208 | 25.633 | 60.274 | 1.00 | 19.21 |
| ATOM | 3116 | CE1 | TYR | B | 113 | 41.902 | 25.283 | 60.002 | 1.00 | 20.32 |
| ATOM | 3117 | CZ  | TYR | B | 113 | 40.871 | 25.942 | 60.626 | 1.00 | 20.68 |
| ATOM | 3118 | OH  | TYR | B | 113 | 39.572 | 25.584 | 60.345 | 1.00 | 24.62 |
| ATOM | 3119 | CE2 | TYR | B | 113 | 41.133 | 26.956 | 61.534 | 1.00 | 14.80 |

**FIGURE 162**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3120 | CD2 | TYR | B | 113 | 42.450 | 27.300 | 61.802 | 1.00 | 15.14 |
| ATOM | 3121 | C   | TYR | B | 113 | 47.090 | 27.916 | 60.726 | 1.00 | 11.85 |
| ATOM | 3122 | O   | TYR | B | 113 | 47.865 | 27.314 | 59.989 | 1.00 | 18.08 |
| ATOM | 3123 | N   | ILE | B | 114 | 47.491 | 28.590 | 61.805 | 1.00 | 17.37 |
| ATOM | 3124 | CA  | ILE | B | 114 | 48.801 | 28.423 | 62.389 | 1.00 | 12.30 |
| ATOM | 3125 | CB  | ILE | B | 114 | 49.576 | 29.751 | 62.490 | 1.00 | 19.28 |
| ATOM | 3126 | CG1 | ILE | B | 114 | 50.011 | 30.240 | 61.102 | 1.00 | 19.55 |
| ATOM | 3127 | CD1 | ILE | B | 114 | 51.019 | 31.347 | 61.037 | 1.00 | 18.32 |
| ATOM | 3128 | CG2 | ILE | B | 114 | 50.722 | 29.619 | 63.473 | 1.00 | 10.43 |
| ATOM | 3129 | C   | ILE | B | 114 | 48.607 | 27.809 | 63.771 | 1.00 | 13.65 |
| ATOM | 3130 | O   | ILE | B | 114 | 47.920 | 28.374 | 64.607 | 1.00 | 20.47 |
| ATOM | 3131 | N   | VAL | B | 115 | 49.207 | 26.630 | 63.960 | 1.00 | 18.21 |
| ATOM | 3132 | CA  | VAL | B | 115 | 49.068 | 25.982 | 65.260 | 1.00 | 21.54 |
| ATOM | 3133 | CB  | VAL | B | 115 | 48.724 | 24.487 | 65.134 | 1.00 | 26.76 |
| ATOM | 3134 | CG1 | VAL | B | 115 | 49.151 | 23.747 | 66.394 | 1.00 | 21.17 |
| ATOM | 3135 | CG2 | VAL | B | 115 | 47.236 | 24.353 | 64.859 | 1.00 | 23.83 |
| ATOM | 3136 | C   | VAL | B | 115 | 50.366 | 26.144 | 66.018 | 1.00 | 15.13 |
| ATOM | 3137 | O   | VAL | B | 115 | 51.470 | 26.092 | 65.484 | 1.00 | 15.47 |
| ATOM | 3138 | N   | THR | B | 116 | 50.255 | 26.378 | 67.328 | 1.00 | 14.92 |
| ATOM | 3139 | CA  | THR | B | 116 | 51.530 | 26.594 | 68.022 | 1.00 | 12.65 |
| ATOM | 3140 | CB  | THR | B | 116 | 51.927 | 28.078 | 67.913 | 1.00 | 16.69 |
| ATOM | 3141 | OG1 | THR | B | 116 | 53.253 | 28.333 | 68.385 | 1.00 | 15.71 |
| ATOM | 3142 | CG2 | THR | B | 116 | 50.956 | 28.910 | 68.764 | 1.00 | 17.43 |
| ATOM | 3143 | C   | THR | B | 116 | 51.360 | 26.112 | 69.463 | 1.00 | 11.03 |
| ATOM | 3144 | O   | THR | B | 116 | 50.246 | 25.848 | 69.902 | 1.00 | 11.09 |
| ATOM | 3145 | N   | GLN | B | 117 | 52.459 | 25.961 | 70.161 | 1.00 | 12.28 |
| ATOM | 3146 | CA  | GLN | B | 117 | 52.444 | 25.635 | 71.579 | 1.00 | 13.83 |
| ATOM | 3147 | CB  | GLN | B | 117 | 53.863 | 25.230 | 71.985 | 1.00 | 14.30 |
| ATOM | 3148 | CG  | GLN | B | 117 | 54.898 | 26.324 | 71.994 | 1.00 | 10.96 |
| ATOM | 3149 | CD  | GLN | B | 117 | 56.300 | 25.936 | 72.377 | 1.00 | 19.11 |
| ATOM | 3150 | OE1 | GLN | B | 117 | 56.676 | 24.759 | 72.435 | 1.00 | 18.55 |
| ATOM | 3151 | NE2 | GLN | B | 117 | 57.164 | 26.915 | 72.649 | 1.00 | 17.68 |
| ATOM | 3152 | C   | GLN | B | 117 | 51.991 | 26.834 | 72.400 | 1.00 | 20.95 |
| ATOM | 3153 | O   | GLN | B | 117 | 52.025 | 27.946 | 71.859 | 1.00 | 14.87 |
| ATOM | 3154 | N   | GLY | B | 118 | 51.630 | 26.648 | 73.666 | 1.00 | 14.16 |
| ATOM | 3155 | CA  | GLY | B | 118 | 51.461 | 27.815 | 74.553 | 1.00 | 11.25 |
| ATOM | 3156 | C   | GLY | B | 118 | 52.809 | 28.483 | 74.732 | 1.00 | 11.67 |
| ATOM | 3157 | O   | GLY | B | 118 | 53.804 | 27.871 | 75.122 | 1.00 | 18.12 |
| ATOM | 3158 | N   | PRO | B | 119 | 52.897 | 29.771 | 74.383 | 1.00 | 15.72 |
| ATOM | 3159 | CA  | PRO | B | 119 | 54.165 | 30.499 | 74.473 | 1.00 | 17.34 |
| ATOM | 3160 | CB  | PRO | B | 119 | 53.761 | 31.941 | 74.150 | 1.00 | 18.05 |
| ATOM | 3161 | CG  | PRO | B | 119 | 52.540 | 31.802 | 73.307 | 1.00 | 16.94 |
| ATOM | 3162 | CD  | PRO | B | 119 | 51.802 | 30.606 | 73.862 | 1.00 | 18.02 |
| ATOM | 3163 | C   | PRO | B | 119 | 54.767 | 30.441 | 75.878 | 1.00 | 12.82 |
| ATOM | 3164 | O   | PRO | B | 119 | 54.020 | 30.432 | 76.865 | 1.00 | 17.29 |
| ATOM | 3165 | N   | LEU | B | 120 | 56.088 | 30.366 | 75.889 | 1.00 | 22.15 |
| ATOM | 3166 | CA  | LEU | B | 120 | 56.900 | 30.382 | 77.094 | 1.00 | 25.66 |
| ATOM | 3167 | CB  | LEU | B | 120 | 58.171 | 29.551 | 76.952 | 1.00 | 21.93 |
| ATOM | 3168 | CG  | LEU | B | 120 | 57.984 | 28.079 | 76.585 | 1.00 | 26.05 |
| ATOM | 3169 | CD1 | LEU | B | 120 | 59.239 | 27.508 | 75.941 | 1.00 | 24.09 |
| ATOM | 3170 | CD2 | LEU | B | 120 | 57.592 | 27.308 | 77.828 | 1.00 | 25.20 |
| ATOM | 3171 | C   | LEU | B | 120 | 57.275 | 31.832 | 77.417 | 1.00 | 23.76 |

**FIGURE 163**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3172 | O   | LEU | B | 120 | 57.201 | 32.682 | 76.533 | 1.00 | 21.98 |
| ATOM | 3173 | N   | PRO | B | 121 | 57.659 | 32.087 | 78.659 | 1.00 | 19.89 |
| ATOM | 3174 | CA  | PRO | B | 121 | 58.151 | 33.418 | 79.028 | 1.00 | 22.32 |
| ATOM | 3175 | CB  | PRO | B | 121 | 58.751 | 33.181 | 80.415 | 1.00 | 25.42 |
| ATOM | 3176 | CG  | PRO | B | 121 | 57.957 | 32.033 | 80.964 | 1.00 | 28.77 |
| ATOM | 3177 | CD  | PRO | B | 121 | 57.648 | 31.145 | 79.793 | 1.00 | 23.68 |
| ATOM | 3178 | C   | PRO | B | 121 | 59.228 | 33.871 | 78.048 | 1.00 | 24.84 |
| ATOM | 3179 | O   | PRO | B | 121 | 59.278 | 35.032 | 77.646 | 1.00 | 28.28 |
| ATOM | 3180 | N   | GLY | B | 122 | 60.083 | 32.929 | 77.647 | 1.00 | 24.79 |
| ATOM | 3181 | CA  | GLY | B | 122 | 61.164 | 33.214 | 76.738 | 1.00 | 26.40 |
| ATOM | 3182 | C   | GLY | B | 122 | 60.850 | 33.227 | 75.260 | 1.00 | 19.61 |
| ATOM | 3183 | O   | GLY | B | 122 | 61.744 | 33.609 | 74.493 | 1.00 | 26.22 |
| ATOM | 3184 | N   | THR | B | 123 | 59.660 | 32.849 | 74.813 | 1.00 | 19.28 |
| ATOM | 3185 | CA  | THR | B | 123 | 59.353 | 32.851 | 73.388 | 1.00 | 21.38 |
| ATOM | 3186 | CB  | THR | B | 123 | 59.009 | 31.450 | 72.839 | 1.00 | 17.49 |
| ATOM | 3187 | OG1 | THR | B | 123 | 57.825 | 30.952 | 73.499 | 1.00 | 18.47 |
| ATOM | 3188 | CG2 | THR | B | 123 | 60.136 | 30.465 | 73.099 | 1.00 | 21.69 |
| ATOM | 3189 | C   | THR | B | 123 | 58.182 | 33.770 | 73.092 | 1.00 | 18.63 |
| ATOM | 3190 | O   | THR | B | 123 | 57.760 | 33.895 | 71.942 | 1.00 | 21.10 |
| ATOM | 3191 | N   | LYS | B | 124 | 57.616 | 34.408 | 74.128 | 1.00 | 17.85 |
| ATOM | 3192 | CA  | LYS | B | 124 | 56.401 | 35.150 | 73.790 | 1.00 | 19.83 |
| ATOM | 3193 | CB  | LYS | B | 124 | 55.659 | 35.684 | 74.999 | 1.00 | 20.67 |
| ATOM | 3194 | CG  | LYS | B | 124 | 56.454 | 36.481 | 76.010 | 1.00 | 22.46 |
| ATOM | 3195 | CD  | LYS | B | 124 | 55.540 | 36.754 | 77.204 | 1.00 | 32.02 |
| ATOM | 3196 | CE  | LYS | B | 124 | 56.234 | 37.523 | 78.317 | 1.00 | 34.93 |
| ATOM | 3197 | NZ  | LYS | B | 124 | 55.312 | 37.592 | 79.499 | 1.00 | 34.71 |
| ATOM | 3198 | C   | LYS | B | 124 | 56.716 | 36.320 | 72.843 | 1.00 | 17.31 |
| ATOM | 3199 | O   | LYS | B | 124 | 55.797 | 36.775 | 72.162 | 1.00 | 18.88 |
| ATOM | 3200 | N   | ASP | B | 125 | 57.972 | 36.753 | 72.843 | 1.00 | 22.11 |
| ATOM | 3201 | CA  | ASP | B | 125 | 58.311 | 37.850 | 71.919 | 1.00 | 32.47 |
| ATOM | 3202 | CB  | ASP | B | 125 | 59.648 | 38.486 | 72.278 | 1.00 | 25.76 |
| ATOM | 3203 | CG  | ASP | B | 125 | 59.590 | 39.330 | 73.544 | 1.00 | 26.93 |
| ATOM | 3204 | OD1 | ASP | B | 125 | 58.487 | 39.534 | 74.093 | 1.00 | 23.69 |
| ATOM | 3205 | OD2 | ASP | B | 125 | 60.656 | 39.797 | 73.994 | 1.00 | 34.33 |
| ATOM | 3206 | C   | ASP | B | 125 | 58.275 | 37.287 | 70.500 | 1.00 | 25.35 |
| ATOM | 3207 | O   | ASP | B | 125 | 57.755 | 37.900 | 69.568 | 1.00 | 20.65 |
| ATOM | 3208 | N   | ASP | B | 126 | 58.823 | 36.085 | 70.361 | 1.00 | 23.45 |
| ATOM | 3209 | CA  | ASP | B | 126 | 58.740 | 35.345 | 69.103 | 1.00 | 28.27 |
| ATOM | 3210 | CB  | ASP | B | 126 | 59.416 | 33.982 | 69.251 | 1.00 | 31.70 |
| ATOM | 3211 | CG  | ASP | B | 126 | 60.912 | 34.025 | 69.453 | 1.00 | 37.78 |
| ATOM | 3212 | OD1 | ASP | B | 126 | 61.567 | 34.998 | 69.021 | 1.00 | 35.70 |
| ATOM | 3213 | OD2 | ASP | B | 126 | 61.452 | 33.065 | 70.055 | 1.00 | 41.12 |
| ATOM | 3214 | C   | ASP | B | 126 | 57.297 | 35.155 | 68.655 | 1.00 | 24.03 |
| ATOM | 3215 | O   | ASP | B | 126 | 56.928 | 35.305 | 67.484 | 1.00 | 21.60 |
| ATOM | 3216 | N   | PHE | B | 127 | 56.418 | 34.780 | 69.586 | 1.00 | 19.45 |
| ATOM | 3217 | CA  | PHE | B | 127 | 55.017 | 34.576 | 69.246 | 1.00 | 18.59 |
| ATOM | 3218 | CB  | PHE | B | 127 | 54.220 | 34.196 | 70.505 | 1.00 | 15.64 |
| ATOM | 3219 | CG  | PHE | B | 127 | 52.714 | 34.146 | 70.345 | 1.00 | 18.56 |
| ATOM | 3220 | CD1 | PHE | B | 127 | 52.137 | 32.939 | 69.936 | 1.00 | 16.99 |
| ATOM | 3221 | CE1 | PHE | B | 127 | 50.771 | 32.846 | 69.790 | 1.00 | 15.74 |
| ATOM | 3222 | CZ  | PHE | B | 127 | 49.941 | 33.925 | 70.023 | 1.00 | 21.60 |
| ATOM | 3223 | CE2 | PHE | B | 127 | 50.506 | 35.127 | 70.433 | 1.00 | 14.92 |

**FIGURE 164**



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3224 | CD2 | PHE | B | 127 | 51.865 | 35.219 | 70.593 | 1.00 | 11.80 |
| ATOM | 3225 | C   | PHE | B | 127 | 54.417 | 35.835 | 68.628 | 1.00 | 15.63 |
| ATOM | 3226 | O   | PHE | B | 127 | 53.711 | 35.819 | 67.627 | 1.00 | 14.92 |
| ATOM | 3227 | N   | TRP | B | 128 | 54.630 | 36.977 | 69.295 | 1.00 | 14.67 |
| ATOM | 3228 | CA  | TRP | B | 128 | 53.959 | 38.186 | 68.805 | 1.00 | 16.59 |
| ATOM | 3229 | CB  | TRP | B | 128 | 53.990 | 39.330 | 69.835 | 1.00 | 14.86 |
| ATOM | 3230 | CG  | TRP | B | 128 | 52.966 | 39.089 | 70.927 | 1.00 | 13.08 |
| ATOM | 3231 | CD1 | TRP | B | 128 | 53.298 | 38.867 | 72.240 | 1.00 | 14.73 |
| ATOM | 3232 | NE1 | TRP | B | 128 | 52.169 | 38.677 | 72.995 | 1.00 | 12.11 |
| ATOM | 3233 | CE2 | TRP | B | 128 | 51.074 | 38.775 | 72.179 | 1.00 | 13.55 |
| ATOM | 3234 | CD2 | TRP | B | 128 | 51.542 | 39.029 | 70.874 | 1.00 | 12.42 |
| ATOM | 3235 | CE3 | TRP | B | 128 | 50.575 | 39.166 | 69.868 | 1.00 | 13.65 |
| ATOM | 3236 | CZ3 | TRP | B | 128 | 49.246 | 39.052 | 70.168 | 1.00 | 19.72 |
| ATOM | 3237 | CH2 | TRP | B | 128 | 48.814 | 38.796 | 71.482 | 1.00 | 22.04 |
| ATOM | 3238 | CZ2 | TRP | B | 128 | 49.725 | 38.655 | 72.495 | 1.00 | 19.42 |
| ATOM | 3239 | C   | TRP | B | 128 | 54.577 | 38.581 | 67.460 | 1.00 | 13.73 |
| ATOM | 3240 | O   | TRP | B | 128 | 53.849 | 39.046 | 66.583 | 1.00 | 22.69 |
| ATOM | 3241 | N   | LYS | B | 129 | 55.877 | 38.373 | 67.292 | 1.00 | 16.55 |
| ATOM | 3242 | CA  | LYS | B | 129 | 56.523 | 38.666 | 66.013 | 1.00 | 19.71 |
| ATOM | 3243 | CB  | LYS | B | 129 | 58.015 | 38.363 | 66.108 | 1.00 | 22.40 |
| ATOM | 3244 | CG  | LYS | B | 129 | 58.811 | 38.769 | 64.883 | 1.00 | 25.13 |
| ATOM | 3245 | CD  | LYS | B | 129 | 60.267 | 38.316 | 64.882 | 1.00 | 28.99 |
| ATOM | 3246 | CE  | LYS | B | 129 | 60.695 | 38.135 | 63.426 | 1.00 | 37.78 |
| ATOM | 3247 | NZ  | LYS | B | 129 | 62.137 | 37.915 | 63.203 | 1.00 | 37.99 |
| ATOM | 3248 | C   | LYS | B | 129 | 55.856 | 37.871 | 64.893 | 1.00 | 32.26 |
| ATOM | 3249 | O   | LYS | B | 129 | 55.560 | 38.383 | 63.811 | 1.00 | 23.65 |
| ATOM | 3250 | N   | MET | B | 130 | 55.586 | 36.593 | 65.147 | 1.00 | 23.24 |
| ATOM | 3251 | CA  | MET | B | 130 | 54.908 | 35.732 | 64.180 | 1.00 | 23.01 |
| ATOM | 3252 | CB  | MET | B | 130 | 54.804 | 34.277 | 64.673 | 1.00 | 20.78 |
| ATOM | 3253 | CG  | MET | B | 130 | 53.968 | 33.376 | 63.751 | 1.00 | 16.92 |
| ATOM | 3254 | SD  | MET | B | 130 | 53.852 | 31.724 | 64.483 | 1.00 | 24.92 |
| ATOM | 3255 | CE  | MET | B | 130 | 52.612 | 31.968 | 65.746 | 1.00 | 15.70 |
| ATOM | 3256 | C   | MET | B | 130 | 53.516 | 36.249 | 63.878 | 1.00 | 16.75 |
| ATOM | 3257 | O   | MET | B | 130 | 53.068 | 36.268 | 62.733 | 1.00 | 21.38 |
| ATOM | 3258 | N   | VAL | B | 131 | 52.799 | 36.648 | 64.923 | 1.00 | 14.58 |
| ATOM | 3259 | CA  | VAL | B | 131 | 51.451 | 37.179 | 64.697 | 1.00 | 11.14 |
| ATOM | 3260 | CB  | VAL | B | 131 | 50.818 | 37.503 | 66.056 | 1.00 | 24.53 |
| ATOM | 3261 | CG1 | VAL | B | 131 | 49.602 | 38.413 | 65.954 | 1.00 | 18.70 |
| ATOM | 3262 | CG2 | VAL | B | 131 | 50.452 | 36.195 | 66.761 | 1.00 | 13.43 |
| ATOM | 3263 | C   | VAL | B | 131 | 51.546 | 38.398 | 63.773 | 1.00 | 16.31 |
| ATOM | 3264 | O   | VAL | B | 131 | 50.746 | 38.556 | 62.845 | 1.00 | 23.18 |
| ATOM | 3265 | N   | TRP | B | 132 | 52.527 | 39.248 | 64.033 | 1.00 | 21.92 |
| ATOM | 3266 | CA  | TRP | B | 132 | 52.707 | 40.480 | 63.256 | 1.00 | 28.19 |
| ATOM | 3267 | CB  | TRP | B | 132 | 53.735 | 41.385 | 63.925 | 1.00 | 16.64 |
| ATOM | 3268 | CG  | TRP | B | 132 | 54.047 | 42.651 | 63.178 | 1.00 | 32.79 |
| ATOM | 3269 | CD1 | TRP | B | 132 | 55.127 | 42.862 | 62.368 | 1.00 | 31.98 |
| ATOM | 3270 | NE1 | TRP | B | 132 | 55.094 | 44.132 | 61.851 | 1.00 | 28.50 |
| ATOM | 3271 | CE2 | TRP | B | 132 | 53.983 | 44.776 | 62.318 | 1.00 | 33.94 |
| ATOM | 3272 | CD2 | TRP | B | 132 | 53.299 | 43.876 | 63.159 | 1.00 | 30.28 |
| ATOM | 3273 | CE3 | TRP | B | 132 | 52.112 | 44.298 | 63.769 | 1.00 | 34.50 |
| ATOM | 3274 | CZ3 | TRP | B | 132 | 51.663 | 45.586 | 63.522 | 1.00 | 38.33 |
| ATOM | 3275 | CH2 | TRP | B | 132 | 52.373 | 46.450 | 62.681 | 1.00 | 35.73 |

**FIGURE 165**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3276 | CZ2 | TRP | B | 132 | 53.535 | 46.073 | 62.065 | 1.00 | 39.63 |
| ATOM | 3277 | C   | TRP | B | 132 | 53.126 | 40.162 | 61.823 | 1.00 | 30.15 |
| ATOM | 3278 | O   | TRP | B | 132 | 52.480 | 40.618 | 60.883 | 1.00 | 22.50 |
| ATOM | 3279 | N   | GLU | B | 133 | 54.185 | 39.377 | 61.636 | 1.00 | 27.59 |
| ATOM | 3280 | CA  | GLU | B | 133 | 54.620 | 39.019 | 60.289 | 1.00 | 24.71 |
| ATOM | 3281 | CB  | GLU | B | 133 | 55.914 | 38.198 | 60.359 | 1.00 | 21.40 |
| ATOM | 3282 | CG  | GLU | B | 133 | 56.932 | 38.826 | 61.304 | 1.00 | 27.89 |
| ATOM | 3283 | CD  | GLU | B | 133 | 58.303 | 38.200 | 61.158 | 1.00 | 32.83 |
| ATOM | 3284 | OE1 | GLU | B | 133 | 58.377 | 36.959 | 61.046 | 1.00 | 36.49 |
| ATOM | 3285 | OE2 | GLU | B | 133 | 59.287 | 38.963 | 61.157 | 1.00 | 38.19 |
| ATOM | 3286 | C   | GLU | B | 133 | 53.583 | 38.245 | 59.492 | 1.00 | 28.74 |
| ATOM | 3287 | O   | GLU | B | 133 | 53.540 | 38.416 | 58.266 | 1.00 | 22.81 |
| ATOM | 3288 | N   | GLN | B | 134 | 52.763 | 37.406 | 60.128 | 1.00 | 20.49 |
| ATOM | 3289 | CA  | GLN | B | 134 | 51.817 | 36.563 | 59.392 | 1.00 | 16.15 |
| ATOM | 3290 | CB  | GLN | B | 134 | 51.619 | 35.216 | 60.088 | 1.00 | 20.39 |
| ATOM | 3291 | CG  | GLN | B | 134 | 52.869 | 34.348 | 60.135 | 1.00 | 23.00 |
| ATOM | 3292 | CD  | GLN | B | 134 | 53.168 | 33.663 | 58.815 | 1.00 | 29.61 |
| ATOM | 3293 | OE1 | GLN | B | 134 | 52.258 | 33.147 | 58.166 | 1.00 | 37.61 |
| ATOM | 3294 | NE2 | GLN | B | 134 | 54.437 | 33.658 | 58.425 | 1.00 | 26.32 |
| ATOM | 3295 | C   | GLN | B | 134 | 50.466 | 37.236 | 59.220 | 1.00 | 19.93 |
| ATOM | 3296 | O   | GLN | B | 134 | 49.519 | 36.586 | 58.783 | 1.00 | 24.92 |
| ATOM | 3297 | N   | ASN | B | 135 | 50.372 | 38.515 | 59.575 | 1.00 | 20.36 |
| ATOM | 3298 | CA  | ASN | B | 135 | 49.118 | 39.244 | 59.402 | 1.00 | 18.42 |
| ATOM | 3299 | CB  | ASN | B | 135 | 48.860 | 39.385 | 57.893 | 1.00 | 28.65 |
| ATOM | 3300 | CG  | ASN | B | 135 | 50.072 | 40.027 | 57.229 | 1.00 | 39.16 |
| ATOM | 3301 | OD1 | ASN | B | 135 | 50.454 | 41.140 | 57.596 | 1.00 | 35.15 |
| ATOM | 3302 | ND2 | ASN | B | 135 | 50.693 | 39.350 | 56.271 | 1.00 | 39.15 |
| ATOM | 3303 | C   | ASN | B | 135 | 47.956 | 38.565 | 60.092 | 1.00 | 21.37 |
| ATOM | 3304 | O   | ASN | B | 135 | 46.828 | 38.506 | 59.609 | 1.00 | 20.97 |
| ATOM | 3305 | N   | VAL | B | 136 | 48.226 | 38.024 | 61.282 | 1.00 | 23.56 |
| ATOM | 3306 | CA  | VAL | B | 136 | 47.159 | 37.346 | 62.021 | 1.00 | 22.94 |
| ATOM | 3307 | CB  | VAL | B | 136 | 47.773 | 36.475 | 63.134 | 1.00 | 19.22 |
| ATOM | 3308 | CG1 | VAL | B | 136 | 46.690 | 35.933 | 64.043 | 1.00 | 20.50 |
| ATOM | 3309 | CG2 | VAL | B | 136 | 48.621 | 35.365 | 62.511 | 1.00 | 13.95 |
| ATOM | 3310 | C   | VAL | B | 136 | 46.210 | 38.363 | 62.640 | 1.00 | 19.65 |
| ATOM | 3311 | O   | VAL | B | 136 | 46.679 | 39.369 | 63.195 | 1.00 | 23.44 |
| ATOM | 3312 | N   | HIS | B | 137 | 44.914 | 38.117 | 62.542 | 1.00 | 15.94 |
| ATOM | 3313 | CA  | HIS | B | 137 | 43.919 | 38.956 | 63.175 | 1.00 | 22.68 |
| ATOM | 3314 | CB  | HIS | B | 137 | 42.921 | 39.537 | 62.162 | 1.00 | 32.34 |
| ATOM | 3315 | CG  | HIS | B | 137 | 43.539 | 40.472 | 61.174 | 1.00 | 50.91 |
| ATOM | 3316 | ND1 | HIS | B | 137 | 42.795 | 41.144 | 60.227 | 1.00 | 62.67 |
| ATOM | 3317 | CE1 | HIS | B | 137 | 43.597 | 41.891 | 59.487 | 1.00 | 61.13 |
| ATOM | 3318 | NE2 | HIS | B | 137 | 44.835 | 41.728 | 59.922 | 1.00 | 55.36 |
| ATOM | 3319 | CD2 | HIS | B | 137 | 44.823 | 40.845 | 60.971 | 1.00 | 46.21 |
| ATOM | 3320 | C   | HIS | B | 137 | 43.129 | 38.192 | 64.237 | 1.00 | 21.18 |
| ATOM | 3321 | O   | HIS | B | 137 | 42.446 | 38.847 | 65.029 | 1.00 | 25.91 |
| ATOM | 3322 | N   | ASN | B | 138 | 43.200 | 36.861 | 64.239 | 1.00 | 20.71 |
| ATOM | 3323 | CA  | ASN | B | 138 | 42.435 | 36.117 | 65.251 | 1.00 | 20.35 |
| ATOM | 3324 | CB  | ASN | B | 138 | 41.167 | 35.466 | 64.683 | 1.00 | 19.57 |
| ATOM | 3325 | CG  | ASN | B | 138 | 40.246 | 36.482 | 64.038 | 1.00 | 25.55 |
| ATOM | 3326 | OD1 | ASN | B | 138 | 40.149 | 36.530 | 62.809 | 1.00 | 32.78 |
| ATOM | 3327 | ND2 | ASN | B | 138 | 39.593 | 37.321 | 64.827 | 1.00 | 15.27 |

**FIGURE 166**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3328 | C   | ASN | B | 138 | 43.316 | 35.057 | 65.905 | 1.00 | 16.32 |
| ATOM | 3329 | O   | ASN | B | 138 | 44.016 | 34.315 | 65.217 | 1.00 | 22.33 |
| ATOM | 3330 | N   | ILE | B | 139 | 43.256 | 35.021 | 67.224 | 1.00 | 12.38 |
| ATOM | 3331 | CA  | ILE | B | 139 | 43.981 | 34.065 | 68.039 | 1.00 | 13.90 |
| ATOM | 3332 | CB  | ILE | B | 139 | 45.010 | 34.736 | 68.966 | 1.00 | 17.37 |
| ATOM | 3333 | CG1 | ILE | B | 139 | 46.050 | 35.606 | 68.246 | 1.00 | 18.49 |
| ATOM | 3334 | CD1 | ILE | B | 139 | 47.007 | 36.323 | 69.166 | 1.00 | 12.78 |
| ATOM | 3335 | CG2 | ILE | B | 139 | 45.702 | 33.693 | 69.832 | 1.00 | 17.74 |
| ATOM | 3336 | C   | ILE | B | 139 | 43.005 | 33.252 | 68.883 | 1.00 | 21.32 |
| ATOM | 3337 | O   | ILE | B | 139 | 42.141 | 33.824 | 69.551 | 1.00 | 17.35 |
| ATOM | 3338 | N   | VAL | B | 140 | 43.161 | 31.923 | 68.805 | 1.00 | 13.24 |
| ATOM | 3339 | CA  | VAL | B | 140 | 42.268 | 31.051 | 69.568 | 1.00 | 16.27 |
| ATOM | 3340 | CB  | VAL | B | 140 | 41.494 | 30.072 | 68.677 | 1.00 | 27.64 |
| ATOM | 3341 | CG1 | VAL | B | 140 | 40.663 | 29.111 | 69.518 | 1.00 | 15.58 |
| ATOM | 3342 | CG2 | VAL | B | 140 | 40.592 | 30.819 | 67.697 | 1.00 | 23.20 |
| ATOM | 3343 | C   | VAL | B | 140 | 43.114 | 30.311 | 70.610 | 1.00 | 18.13 |
| ATOM | 3344 | O   | VAL | B | 140 | 44.176 | 29.761 | 70.291 | 1.00 | 14.05 |
| ATOM | 3345 | N   | MET | B | 141 | 42.658 | 30.324 | 71.870 | 1.00 | 13.85 |
| ATOM | 3346 | CA  | MET | B | 141 | 43.424 | 29.744 | 72.969 | 1.00 | 17.23 |
| ATOM | 3347 | CB  | MET | B | 141 | 43.894 | 30.844 | 73.939 | 1.00 | 16.81 |
| ATOM | 3348 | CG  | MET | B | 141 | 44.730 | 30.340 | 75.094 | 1.00 | 16.69 |
| ATOM | 3349 | SD  | MET | B | 141 | 45.484 | 31.660 | 76.071 | 1.00 | 18.21 |
| ATOM | 3350 | CE  | MET | B | 141 | 46.209 | 30.676 | 77.403 | 1.00 | 22.43 |
| ATOM | 3351 | C   | MET | B | 141 | 42.539 | 28.740 | 73.681 | 1.00 | 18.04 |
| ATOM | 3352 | O   | MET | B | 141 | 41.502 | 29.159 | 74.204 | 1.00 | 23.03 |
| ATOM | 3353 | N   | VAL | B | 142 | 42.894 | 27.450 | 73.708 | 1.00 | 13.36 |
| ATOM | 3354 | CA  | VAL | B | 142 | 41.913 | 26.540 | 74.325 | 1.00 | 13.57 |
| ATOM | 3355 | CB  | VAL | B | 142 | 41.368 | 25.488 | 73.342 | 1.00 | 16.78 |
| ATOM | 3356 | CG1 | VAL | B | 142 | 40.352 | 26.126 | 72.403 | 1.00 | 25.66 |
| ATOM | 3357 | CG2 | VAL | B | 142 | 42.526 | 24.857 | 72.591 | 1.00 | 22.06 |
| ATOM | 3358 | C   | VAL | B | 142 | 42.536 | 25.823 | 75.513 | 1.00 | 15.54 |
| ATOM | 3359 | O   | VAL | B | 142 | 42.224 | 24.690 | 75.854 | 1.00 | 36.13 |
| ATOM | 3360 | N   | THR | B | 143 | 43.443 | 26.538 | 76.161 | 1.00 | 19.81 |
| ATOM | 3361 | CA  | THR | B | 143 | 44.013 | 26.054 | 77.415 | 1.00 | 23.30 |
| ATOM | 3362 | CB  | THR | B | 143 | 45.474 | 25.625 | 77.268 | 1.00 | 20.98 |
| ATOM | 3363 | OG1 | THR | B | 143 | 45.916 | 24.941 | 78.455 | 1.00 | 20.64 |
| ATOM | 3364 | CG2 | THR | B | 143 | 46.363 | 26.856 | 77.104 | 1.00 | 18.59 |
| ATOM | 3365 | C   | THR | B | 143 | 43.915 | 27.174 | 78.445 | 1.00 | 27.90 |
| ATOM | 3366 | O   | THR | B | 143 | 43.801 | 28.343 | 78.083 | 1.00 | 18.82 |
| ATOM | 3367 | N   | GLN | B | 144 | 43.972 | 26.814 | 79.720 | 1.00 | 24.18 |
| ATOM | 3368 | CA  | GLN | B | 144 | 44.194 | 27.849 | 80.726 | 1.00 | 26.49 |
| ATOM | 3369 | CB  | GLN | B | 144 | 43.490 | 27.554 | 82.038 | 1.00 | 25.93 |
| ATOM | 3370 | CG  | GLN | B | 144 | 41.973 | 27.692 | 81.972 | 1.00 | 31.81 |
| ATOM | 3371 | CD  | GLN | B | 144 | 41.409 | 27.232 | 83.315 | 1.00 | 43.70 |
| ATOM | 3372 | OE1 | GLN | B | 144 | 41.157 | 28.059 | 84.185 | 1.00 | 50.17 |
| ATOM | 3373 | NE2 | GLN | B | 144 | 41.251 | 25.923 | 83.447 | 1.00 | 42.17 |
| ATOM | 3374 | C   | GLN | B | 144 | 45.701 | 27.911 | 80.950 | 1.00 | 21.88 |
| ATOM | 3375 | O   | GLN | B | 144 | 46.371 | 26.926 | 80.618 | 1.00 | 18.20 |
| ATOM | 3376 | N   | CYS | B | 145 | 46.176 | 29.017 | 81.502 | 1.00 | 17.45 |
| ATOM | 3377 | CA  | CYS | B | 145 | 47.594 | 29.207 | 81.718 | 1.00 | 13.43 |
| ATOM | 3378 | CB  | CYS | B | 145 | 47.853 | 30.629 | 82.221 | 1.00 | 20.41 |
| ATOM | 3379 | SG  | CYS | B | 145 | 47.629 | 31.851 | 80.891 | 1.00 | 23.38 |

**FIGURE 167**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3380 | C   | CYS | B | 145 | 48.151 | 28.198 | 82.726 | 1.00 | 13.94 |
| ATOM | 3381 | O   | CYS | B | 145 | 49.278 | 27.738 | 82.611 | 1.00 | 14.73 |
| ATOM | 3382 | N   | VAL | B | 146 | 47.320 | 27.912 | 83.716 | 1.00 | 19.10 |
| ATOM | 3383 | CA  | VAL | B | 146 | 47.674 | 26.994 | 84.798 | 1.00 | 21.25 |
| ATOM | 3384 | CB  | VAL | B | 146 | 48.116 | 27.718 | 86.081 | 1.00 | 23.42 |
| ATOM | 3385 | CG1 | VAL | B | 146 | 48.515 | 26.713 | 87.163 | 1.00 | 17.61 |
| ATOM | 3386 | CG2 | VAL | B | 146 | 49.270 | 28.661 | 85.793 | 1.00 | 20.80 |
| ATOM | 3387 | C   | VAL | B | 146 | 46.449 | 26.145 | 85.081 | 1.00 | 19.88 |
| ATOM | 3388 | O   | VAL | B | 146 | 45.355 | 26.702 | 85.219 | 1.00 | 21.18 |
| ATOM | 3389 | N   | GLU | B | 147 | 46.590 | 24.824 | 85.132 | 1.00 | 18.68 |
| ATOM | 3390 | CA  | GLU | B | 147 | 45.398 | 24.012 | 85.422 | 1.00 | 18.49 |
| ATOM | 3391 | CB  | GLU | B | 147 | 45.048 | 23.119 | 84.225 | 1.00 | 21.59 |
| ATOM | 3392 | CG  | GLU | B | 147 | 44.374 | 23.905 | 83.116 | 1.00 | 23.43 |
| ATOM | 3393 | CD  | GLU | B | 147 | 44.162 | 23.234 | 81.785 | 1.00 | 38.61 |
| ATOM | 3394 | OE1 | GLU | B | 147 | 44.493 | 22.040 | 81.618 | 1.00 | 34.89 |
| ATOM | 3395 | OE2 | GLU | B | 147 | 43.636 | 23.926 | 80.870 | 1.00 | 30.39 |
| ATOM | 3396 | C   | GLU | B | 147 | 45.675 | 23.194 | 86.675 | 1.00 | 22.32 |
| ATOM | 3397 | O   | GLU | B | 147 | 46.589 | 22.361 | 86.632 | 1.00 | 27.28 |
| ATOM | 3398 | N   | LYS | B | 148 | 44.956 | 23.423 | 87.767 | 1.00 | 30.22 |
| ATOM | 3399 | CA  | LYS | B | 148 | 45.226 | 22.630 | 88.976 | 1.00 | 32.97 |
| ATOM | 3400 | CB  | LYS | B | 148 | 44.850 | 21.169 | 88.720 | 1.00 | 39.67 |
| ATOM | 3401 | CG  | LYS | B | 148 | 43.346 | 20.947 | 88.598 | 1.00 | 44.29 |
| ATOM | 3402 | CD  | LYS | B | 148 | 43.029 | 19.958 | 87.489 | 1.00 | 44.33 |
| ATOM | 3403 | CE  | LYS | B | 148 | 41.527 | 19.780 | 87.325 | 1.00 | 49.46 |
| ATOM | 3404 | NZ  | LYS | B | 148 | 41.028 | 20.351 | 86.043 | 1.00 | 61.43 |
| ATOM | 3405 | C   | LYS | B | 148 | 46.681 | 22.757 | 89.395 | 1.00 | 28.17 |
| ATOM | 3406 | O   | LYS | B | 148 | 47.401 | 21.830 | 89.761 | 1.00 | 28.44 |
| ATOM | 3407 | N   | GLY | B | 149 | 47.163 | 24.001 | 89.303 | 1.00 | 19.82 |
| ATOM | 3408 | CA  | GLY | B | 149 | 48.533 | 24.259 | 89.642 | 1.00 | 14.78 |
| ATOM | 3409 | C   | GLY | B | 149 | 49.550 | 23.826 | 88.611 | 1.00 | 25.79 |
| ATOM | 3410 | O   | GLY | B | 149 | 50.723 | 24.180 | 88.775 | 1.00 | 24.43 |
| ATOM | 3411 | N   | ARG | B | 150 | 49.192 | 23.090 | 87.559 | 1.00 | 24.49 |
| ATOM | 3412 | CA  | ARG | B | 150 | 50.193 | 22.668 | 86.579 | 1.00 | 21.93 |
| ATOM | 3413 | CB  | ARG | B | 150 | 49.803 | 21.317 | 85.965 | 1.00 | 24.07 |
| ATOM | 3414 | CG  | ARG | B | 150 | 49.775 | 20.179 | 86.980 | 1.00 | 28.42 |
| ATOM | 3415 | CD  | ARG | B | 150 | 49.328 | 18.870 | 86.341 | 1.00 | 38.83 |
| ATOM | 3416 | NE  | ARG | B | 150 | 48.126 | 18.371 | 87.014 | 1.00 | 49.80 |
| ATOM | 3417 | CZ  | ARG | B | 150 | 46.904 | 18.817 | 86.738 | 1.00 | 54.11 |
| ATOM | 3418 | NH1 | ARG | B | 150 | 46.718 | 19.752 | 85.811 | 1.00 | 48.84 |
| ATOM | 3419 | NH2 | ARG | B | 150 | 45.865 | 18.319 | 87.394 | 1.00 | 45.18 |
| ATOM | 3420 | C   | ARG | B | 150 | 50.346 | 23.708 | 85.467 | 1.00 | 15.49 |
| ATOM | 3421 | O   | ARG | B | 150 | 49.325 | 24.039 | 84.872 | 1.00 | 23.49 |
| ATOM | 3422 | N   | VAL | B | 151 | 51.543 | 24.202 | 85.215 | 1.00 | 18.22 |
| ATOM | 3423 | CA  | VAL | B | 151 | 51.760 | 25.224 | 84.188 | 1.00 | 20.43 |
| ATOM | 3424 | CB  | VAL | B | 151 | 53.188 | 25.789 | 84.283 | 1.00 | 27.81 |
| ATOM | 3425 | CG1 | VAL | B | 151 | 53.440 | 26.853 | 83.216 | 1.00 | 35.66 |
| ATOM | 3426 | CG2 | VAL | B | 151 | 53.439 | 26.378 | 85.667 | 1.00 | 24.07 |
| ATOM | 3427 | C   | VAL | B | 151 | 51.513 | 24.667 | 82.790 | 1.00 | 23.20 |
| ATOM | 3428 | O   | VAL | B | 151 | 52.059 | 23.622 | 82.440 | 1.00 | 19.63 |
| ATOM | 3429 | N   | LYS | B | 152 | 50.707 | 25.370 | 82.006 | 1.00 | 24.64 |
| ATOM | 3430 | CA  | LYS | B | 152 | 50.357 | 24.963 | 80.651 | 1.00 | 14.29 |
| ATOM | 3431 | CB  | LYS | B | 152 | 48.860 | 24.691 | 80.517 | 1.00 | 10.40 |

**FIGURE 168**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3432 | CG  | LYS | B | 152 | 48.253 | 23.776 | 81.578 | 1.00 | 17.03 |
| ATOM | 3433 | CD  | LYS | B | 152 | 48.788 | 22.349 | 81.417 | 1.00 | 21.83 |
| ATOM | 3434 | CE  | LYS | B | 152 | 47.958 | 21.386 | 82.264 | 1.00 | 22.06 |
| ATOM | 3435 | NZ  | LYS | B | 152 | 48.298 | 19.972 | 81.959 | 1.00 | 36.68 |
| ATOM | 3436 | C   | LYS | B | 152 | 50.754 | 26.040 | 79.644 | 1.00 | 24.64 |
| ATOM | 3437 | O   | LYS | B | 152 | 51.009 | 25.763 | 78.468 | 1.00 | 18.65 |
| ATOM | 3438 | N   | CYS | B | 153 | 50.803 | 27.314 | 80.047 | 1.00 | 11.48 |
| ATOM | 3439 | CA  | CYS | B | 153 | 51.051 | 28.334 | 79.016 | 1.00 | 12.40 |
| ATOM | 3440 | CB  | CYS | B | 153 | 49.804 | 28.484 | 78.135 | 1.00 | 12.34 |
| ATOM | 3441 | SG  | CYS | B | 153 | 49.930 | 29.808 | 76.878 | 1.00 | 18.57 |
| ATOM | 3442 | C   | CYS | B | 153 | 51.402 | 29.647 | 79.697 | 1.00 | 21.82 |
| ATOM | 3443 | O   | CYS | B | 153 | 50.893 | 29.972 | 80.777 | 1.00 | 18.60 |
| ATOM | 3444 | N   | ASP | B | 154 | 52.295 | 30.439 | 79.135 | 1.00 | 16.73 |
| ATOM | 3445 | CA  | ASP | B | 154 | 52.588 | 31.722 | 79.807 | 1.00 | 16.66 |
| ATOM | 3446 | CB  | ASP | B | 154 | 53.893 | 32.268 | 79.253 | 1.00 | 17.86 |
| ATOM | 3447 | CG  | ASP | B | 154 | 54.346 | 33.504 | 80.006 | 1.00 | 28.26 |
| ATOM | 3448 | OD1 | ASP | B | 154 | 54.311 | 34.561 | 79.347 | 1.00 | 32.47 |
| ATOM | 3449 | OD2 | ASP | B | 154 | 54.693 | 33.396 | 81.199 | 1.00 | 26.75 |
| ATOM | 3450 | C   | ASP | B | 154 | 51.417 | 32.676 | 79.644 | 1.00 | 19.16 |
| ATOM | 3451 | O   | ASP | B | 154 | 50.633 | 32.566 | 78.696 | 1.00 | 19.76 |
| ATOM | 3452 | N   | HIS | B | 155 | 51.254 | 33.609 | 80.583 | 1.00 | 18.37 |
| ATOM | 3453 | CA  | HIS | B | 155 | 50.258 | 34.666 | 80.434 | 1.00 | 19.93 |
| ATOM | 3454 | CB  | HIS | B | 155 | 49.911 | 35.303 | 81.787 | 1.00 | 13.95 |
| ATOM | 3455 | CG  | HIS | B | 155 | 48.744 | 36.236 | 81.679 | 1.00 | 17.38 |
| ATOM | 3456 | ND1 | HIS | B | 155 | 47.470 | 35.952 | 82.137 | 1.00 | 21.90 |
| ATOM | 3457 | CE1 | HIS | B | 155 | 46.665 | 36.975 | 81.889 | 1.00 | 23.51 |
| ATOM | 3458 | NE2 | HIS | B | 155 | 47.376 | 37.912 | 81.278 | 1.00 | 25.28 |
| ATOM | 3459 | CD2 | HIS | B | 155 | 48.669 | 37.476 | 81.135 | 1.00 | 15.32 |
| ATOM | 3460 | C   | HIS | B | 155 | 50.871 | 35.672 | 79.468 | 1.00 | 23.82 |
| ATOM | 3461 | O   | HIS | B | 155 | 51.437 | 36.664 | 79.913 | 1.00 | 26.73 |
| ATOM | 3462 | N   | TYR | B | 156 | 50.820 | 35.411 | 78.158 | 1.00 | 12.99 |
| ATOM | 3463 | CA  | TYR | B | 156 | 51.669 | 36.173 | 77.258 | 1.00 | 17.64 |
| ATOM | 3464 | CB  | TYR | B | 156 | 51.996 | 35.306 | 76.025 | 1.00 | 17.34 |
| ATOM | 3465 | CG  | TYR | B | 156 | 50.780 | 34.829 | 75.270 | 1.00 | 14.33 |
| ATOM | 3466 | CD1 | TYR | B | 156 | 50.206 | 35.541 | 74.233 | 1.00 | 9.88  |
| ATOM | 3467 | CE1 | TYR | B | 156 | 49.095 | 35.057 | 73.566 | 1.00 | 17.37 |
| ATOM | 3468 | CZ  | TYR | B | 156 | 48.537 | 33.843 | 73.912 | 1.00 | 16.91 |
| ATOM | 3469 | OH  | TYR | B | 156 | 47.427 | 33.352 | 73.252 | 1.00 | 16.15 |
| ATOM | 3470 | CE2 | TYR | B | 156 | 49.095 | 33.107 | 74.941 | 1.00 | 16.17 |
| ATOM | 3471 | CD2 | TYR | B | 156 | 50.202 | 33.597 | 75.603 | 1.00 | 19.17 |
| ATOM | 3472 | C   | TYR | B | 156 | 51.099 | 37.488 | 76.740 | 1.00 | 15.11 |
| ATOM | 3473 | O   | TYR | B | 156 | 51.731 | 38.066 | 75.839 | 1.00 | 17.69 |
| ATOM | 3474 | N   | TRP | B | 157 | 49.973 | 37.913 | 77.257 | 1.00 | 20.44 |
| ATOM | 3475 | CA  | TRP | B | 157 | 49.317 | 39.185 | 76.948 | 1.00 | 22.51 |
| ATOM | 3476 | CB  | TRP | B | 157 | 47.941 | 38.916 | 76.355 | 1.00 | 19.87 |
| ATOM | 3477 | CG  | TRP | B | 157 | 46.985 | 38.298 | 77.330 | 1.00 | 19.72 |
| ATOM | 3478 | CD1 | TRP | B | 157 | 46.114 | 38.986 | 78.133 | 1.00 | 21.12 |
| ATOM | 3479 | NE1 | TRP | B | 157 | 45.393 | 38.102 | 78.898 | 1.00 | 21.03 |
| ATOM | 3480 | CE2 | TRP | B | 157 | 45.787 | 36.823 | 78.596 | 1.00 | 22.01 |
| ATOM | 3481 | CD2 | TRP | B | 157 | 46.788 | 36.910 | 77.612 | 1.00 | 21.27 |
| ATOM | 3482 | CE3 | TRP | B | 157 | 47.353 | 35.722 | 77.140 | 1.00 | 15.87 |
| ATOM | 3483 | CZ3 | TRP | B | 157 | 46.911 | 34.519 | 77.650 | 1.00 | 21.70 |

**FIGURE 169**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3484 | CH2 | TRP | B | 157 | 45.909 | 34.468 | 78.629 | 1.00 | 22.88 |
| ATOM | 3485 | CZ2 | TRP | B | 157 | 45.339 | 35.614 | 79.114 | 1.00 | 25.47 |
| ATOM | 3486 | C   | TRP | B | 157 | 49.245 | 40.010 | 78.227 | 1.00 | 31.95 |
| ATOM | 3487 | O   | TRP | B | 157 | 49.455 | 39.413 | 79.292 | 1.00 | 26.71 |
| ATOM | 3488 | N   | PRO | B | 158 | 48.992 | 41.310 | 78.208 | 1.00 | 31.73 |
| ATOM | 3489 | CA  | PRO | B | 158 | 49.055 | 42.131 | 79.423 | 1.00 | 27.67 |
| ATOM | 3490 | CB  | PRO | B | 158 | 48.882 | 43.564 | 78.893 | 1.00 | 33.72 |
| ATOM | 3491 | CG  | PRO | B | 158 | 49.181 | 43.472 | 77.432 | 1.00 | 33.76 |
| ATOM | 3492 | CD  | PRO | B | 158 | 48.645 | 42.119 | 77.021 | 1.00 | 35.38 |
| ATOM | 3493 | C   | PRO | B | 158 | 47.944 | 41.845 | 80.427 | 1.00 | 34.39 |
| ATOM | 3494 | O   | PRO | B | 158 | 46.852 | 41.408 | 80.064 | 1.00 | 43.08 |
| ATOM | 3495 | N   | ALA | B | 159 | 48.213 | 42.100 | 81.706 | 1.00 | 42.13 |
| ATOM | 3496 | CA  | ALA | B | 159 | 47.276 | 41.840 | 82.796 | 1.00 | 36.27 |
| ATOM | 3497 | CB  | ALA | B | 159 | 47.929 | 42.175 | 84.134 | 1.00 | 24.16 |
| ATOM | 3498 | C   | ALA | B | 159 | 45.986 | 42.624 | 82.659 | 1.00 | 36.43 |
| ATOM | 3499 | O   | ALA | B | 159 | 44.871 | 42.160 | 82.889 | 1.00 | 36.44 |
| ATOM | 3500 | N   | ASP | B | 160 | 46.124 | 43.889 | 82.264 | 1.00 | 30.03 |
| ATOM | 3501 | CA  | ASP | B | 160 | 44.940 | 44.748 | 82.237 | 1.00 | 35.84 |
| ATOM | 3502 | CB  | ASP | B | 160 | 44.838 | 45.506 | 83.566 | 1.00 | 38.86 |
| ATOM | 3503 | CG  | ASP | B | 160 | 46.127 | 46.268 | 83.835 | 1.00 | 40.84 |
| ATOM | 3504 | OD1 | ASP | B | 160 | 46.496 | 47.091 | 82.969 | 1.00 | 44.84 |
| ATOM | 3505 | OD2 | ASP | B | 160 | 46.760 | 46.038 | 84.883 | 1.00 | 45.44 |
| ATOM | 3506 | C   | ASP | B | 160 | 45.033 | 45.682 | 81.045 | 1.00 | 34.03 |
| ATOM | 3507 | O   | ASP | B | 160 | 45.484 | 45.251 | 79.981 | 1.00 | 35.16 |
| ATOM | 3508 | N   | GLN | B | 161 | 44.646 | 46.947 | 81.174 | 1.00 | 31.44 |
| ATOM | 3509 | CA  | GLN | B | 161 | 44.665 | 47.795 | 79.971 | 1.00 | 37.31 |
| ATOM | 3510 | CB  | GLN | B | 161 | 43.443 | 48.713 | 79.958 | 1.00 | 48.77 |
| ATOM | 3511 | CG  | GLN | B | 161 | 42.113 | 48.002 | 80.141 | 1.00 | 63.63 |
| ATOM | 3512 | CD  | GLN | B | 161 | 41.545 | 47.351 | 78.898 | 1.00 | 66.46 |
| ATOM | 3513 | OE1 | GLN | B | 161 | 41.702 | 47.819 | 77.769 | 1.00 | 73.28 |
| ATOM | 3514 | NE2 | GLN | B | 161 | 40.851 | 46.230 | 79.085 | 1.00 | 44.47 |
| ATOM | 3515 | C   | GLN | B | 161 | 45.959 | 48.574 | 79.868 | 1.00 | 30.80 |
| ATOM | 3516 | O   | GLN | B | 161 | 46.164 | 49.414 | 78.991 | 1.00 | 30.61 |
| ATOM | 3517 | N   | ASP | B | 162 | 46.927 | 48.325 | 80.752 | 1.00 | 31.03 |
| ATOM | 3518 | CA  | ASP | B | 162 | 48.201 | 49.018 | 80.507 | 1.00 | 39.93 |
| ATOM | 3519 | CB  | ASP | B | 162 | 49.077 | 49.016 | 81.756 | 1.00 | 50.93 |
| ATOM | 3520 | CG  | ASP | B | 162 | 49.441 | 47.616 | 82.213 | 1.00 | 68.18 |
| ATOM | 3521 | OD1 | ASP | B | 162 | 48.998 | 46.637 | 81.574 | 1.00 | 86.94 |
| ATOM | 3522 | OD2 | ASP | B | 162 | 50.176 | 47.492 | 83.218 | 1.00 | 99.89 |
| ATOM | 3523 | C   | ASP | B | 162 | 48.904 | 48.357 | 79.324 | 1.00 | 39.36 |
| ATOM | 3524 | O   | ASP | B | 162 | 48.627 | 47.197 | 79.014 | 1.00 | 54.50 |
| ATOM | 3525 | N   | SER | B | 163 | 49.796 | 49.081 | 78.659 | 1.00 | 29.38 |
| ATOM | 3526 | CA  | SER | B | 163 | 50.522 | 48.555 | 77.510 | 1.00 | 24.30 |
| ATOM | 3527 | CB  | SER | B | 163 | 50.671 | 49.686 | 76.476 | 1.00 | 24.27 |
| ATOM | 3528 | OG  | SER | B | 163 | 51.323 | 50.772 | 77.118 | 1.00 | 33.50 |
| ATOM | 3529 | C   | SER | B | 163 | 51.887 | 47.999 | 77.867 | 1.00 | 27.40 |
| ATOM | 3530 | O   | SER | B | 163 | 52.500 | 48.320 | 78.886 | 1.00 | 30.35 |
| ATOM | 3531 | N   | LEU | B | 164 | 52.412 | 47.131 | 77.004 | 1.00 | 22.69 |
| ATOM | 3532 | CA  | LEU | B | 164 | 53.721 | 46.549 | 77.197 | 1.00 | 23.41 |
| ATOM | 3533 | CB  | LEU | B | 164 | 53.666 | 45.205 | 77.926 | 1.00 | 32.71 |
| ATOM | 3534 | CG  | LEU | B | 164 | 53.276 | 45.168 | 79.401 | 1.00 | 41.07 |
| ATOM | 3535 | CD1 | LEU | B | 164 | 52.777 | 43.780 | 79.796 | 1.00 | 39.52 |

**FIGURE 170**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3536 | CD2 | LEU | B | 164 | 54.432 | 45.565 | 80.311 | 1.00 | 34.59 |
| ATOM | 3537 | C   | LEU | B | 164 | 54.400 | 46.334 | 75.839 | 1.00 | 19.77 |
| ATOM | 3538 | O   | LEU | B | 164 | 53.727 | 46.182 | 74.820 | 1.00 | 25.31 |
| ATOM | 3539 | N   | TYR | B | 165 | 55.717 | 46.327 | 75.881 | 1.00 | 22.94 |
| ATOM | 3540 | CA  | TYR | B | 165 | 56.537 | 45.961 | 74.752 | 1.00 | 22.36 |
| ATOM | 3541 | CB  | TYR | B | 165 | 57.888 | 46.643 | 74.765 | 1.00 | 18.40 |
| ATOM | 3542 | CG  | TYR | B | 165 | 57.974 | 48.100 | 74.409 | 1.00 | 29.19 |
| ATOM | 3543 | CD1 | TYR | B | 165 | 57.965 | 49.067 | 75.410 | 1.00 | 33.88 |
| ATOM | 3544 | CE1 | TYR | B | 165 | 58.049 | 50.410 | 75.103 | 1.00 | 30.20 |
| ATOM | 3545 | CZ  | TYR | B | 165 | 58.150 | 50.803 | 73.792 | 1.00 | 29.95 |
| ATOM | 3546 | OH  | TYR | B | 165 | 58.232 | 52.144 | 73.492 | 1.00 | 23.81 |
| ATOM | 3547 | CE2 | TYR | B | 165 | 58.167 | 49.866 | 72.780 | 1.00 | 32.37 |
| ATOM | 3548 | CD2 | TYR | B | 165 | 58.082 | 48.525 | 73.091 | 1.00 | 29.59 |
| ATOM | 3549 | C   | TYR | B | 165 | 56.812 | 44.448 | 74.759 | 1.00 | 28.65 |
| ATOM | 3550 | O   | TYR | B | 165 | 57.094 | 43.855 | 75.793 | 1.00 | 27.24 |
| ATOM | 3551 | N   | TYR | B | 166 | 56.752 | 43.893 | 73.562 | 1.00 | 26.38 |
| ATOM | 3552 | CA  | TYR | B | 166 | 57.169 | 42.527 | 73.276 | 1.00 | 23.90 |
| ATOM | 3553 | CB  | TYR | B | 166 | 55.962 | 41.650 | 73.008 | 1.00 | 20.88 |
| ATOM | 3554 | CG  | TYR | B | 166 | 54.973 | 41.508 | 74.140 | 1.00 | 22.61 |
| ATOM | 3555 | CD1 | TYR | B | 166 | 55.113 | 40.482 | 75.076 | 1.00 | 21.82 |
| ATOM | 3556 | CE1 | TYR | B | 166 | 54.199 | 40.362 | 76.101 | 1.00 | 17.08 |
| ATOM | 3557 | CZ  | TYR | B | 166 | 53.148 | 41.235 | 76.224 | 1.00 | 19.26 |
| ATOM | 3558 | OH  | TYR | B | 166 | 52.255 | 41.100 | 77.248 | 1.00 | 19.82 |
| ATOM | 3559 | CE2 | TYR | B | 166 | 52.976 | 42.262 | 75.313 | 1.00 | 22.80 |
| ATOM | 3560 | CD2 | TYR | B | 166 | 53.901 | 42.367 | 74.291 | 1.00 | 23.91 |
| ATOM | 3561 | C   | TYR | B | 166 | 58.105 | 42.598 | 72.069 | 1.00 | 15.01 |
| ATOM | 3562 | O   | TYR | B | 166 | 57.616 | 42.676 | 70.943 | 1.00 | 23.20 |
| ATOM | 3563 | N   | GLY | B | 167 | 59.399 | 42.596 | 72.328 | 1.00 | 23.31 |
| ATOM | 3564 | CA  | GLY | B | 167 | 60.399 | 42.819 | 71.301 | 1.00 | 30.99 |
| ATOM | 3565 | C   | GLY | B | 167 | 60.278 | 44.237 | 70.754 | 1.00 | 32.92 |
| ATOM | 3566 | O   | GLY | B | 167 | 60.252 | 45.223 | 71.498 | 1.00 | 31.28 |
| ATOM | 3567 | N   | ASP | B | 168 | 60.195 | 44.348 | 69.432 | 1.00 | 24.47 |
| ATOM | 3568 | CA  | ASP | B | 168 | 60.036 | 45.656 | 68.810 | 1.00 | 30.37 |
| ATOM | 3569 | CB  | ASP | B | 168 | 60.661 | 45.694 | 67.414 | 1.00 | 35.10 |
| ATOM | 3570 | CG  | ASP | B | 168 | 62.142 | 45.378 | 67.460 | 1.00 | 42.09 |
| ATOM | 3571 | OD1 | ASP | B | 168 | 62.723 | 45.550 | 68.550 | 1.00 | 47.47 |
| ATOM | 3572 | OD2 | ASP | B | 168 | 62.684 | 44.966 | 66.414 | 1.00 | 47.31 |
| ATOM | 3573 | C   | ASP | B | 168 | 58.570 | 46.022 | 68.666 | 1.00 | 29.02 |
| ATOM | 3574 | O   | ASP | B | 168 | 58.240 | 46.976 | 67.967 | 1.00 | 37.58 |
| ATOM | 3575 | N   | LEU | B | 169 | 57.674 | 45.259 | 69.296 | 1.00 | 24.88 |
| ATOM | 3576 | CA  | LEU | B | 169 | 56.265 | 45.583 | 69.132 | 1.00 | 19.15 |
| ATOM | 3577 | CB  | LEU | B | 169 | 55.436 | 44.377 | 68.702 | 1.00 | 29.37 |
| ATOM | 3578 | CG  | LEU | B | 169 | 55.736 | 43.693 | 67.375 | 1.00 | 33.58 |
| ATOM | 3579 | CD1 | LEU | B | 169 | 55.206 | 42.262 | 67.367 | 1.00 | 22.11 |
| ATOM | 3580 | CD2 | LEU | B | 169 | 55.145 | 44.492 | 66.220 | 1.00 | 40.24 |
| ATOM | 3581 | C   | LEU | B | 169 | 55.705 | 46.081 | 70.461 | 1.00 | 18.08 |
| ATOM | 3582 | O   | LEU | B | 169 | 56.260 | 45.744 | 71.498 | 1.00 | 30.36 |
| ATOM | 3583 | N   | ILE | B | 170 | 54.625 | 46.828 | 70.374 | 1.00 | 23.85 |
| ATOM | 3584 | CA  | ILE | B | 170 | 53.900 | 47.229 | 71.571 | 1.00 | 29.93 |
| ATOM | 3585 | CB  | ILE | B | 170 | 53.947 | 48.744 | 71.817 | 1.00 | 31.71 |
| ATOM | 3586 | CG1 | ILE | B | 170 | 53.316 | 49.167 | 73.144 | 1.00 | 36.34 |
| ATOM | 3587 | CD1 | ILE | B | 170 | 54.269 | 49.867 | 74.084 | 1.00 | 48.77 |

**FIGURE 171**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3588 | CG2 | ILE | B | 170 | 53.304 | 49.482 | 70.662 | 1.00 | 37.89 |
| ATOM | 3589 | C   | ILE | B | 170 | 52.460 | 46.757 | 71.433 | 1.00 | 30.07 |
| ATOM | 3590 | O   | ILE | B | 170 | 51.841 | 46.853 | 70.374 | 1.00 | 29.12 |
| ATOM | 3591 | N   | LEU | B | 171 | 51.955 | 46.223 | 72.535 | 1.00 | 25.46 |
| ATOM | 3592 | CA  | LEU | B | 171 | 50.604 | 45.701 | 72.589 | 1.00 | 21.46 |
| ATOM | 3593 | CB  | LEU | B | 171 | 50.612 | 44.200 | 72.895 | 1.00 | 29.41 |
| ATOM | 3594 | CG  | LEU | B | 171 | 50.226 | 43.287 | 71.727 | 1.00 | 39.01 |
| ATOM | 3595 | CD1 | LEU | B | 171 | 51.391 | 43.140 | 70.758 | 1.00 | 43.97 |
| ATOM | 3596 | CD2 | LEU | B | 171 | 49.774 | 41.940 | 72.246 | 1.00 | 47.22 |
| ATOM | 3597 | C   | LEU | B | 171 | 49.805 | 46.423 | 73.668 | 1.00 | 25.20 |
| ATOM | 3598 | O   | LEU | B | 171 | 50.337 | 46.746 | 74.734 | 1.00 | 26.76 |
| ATOM | 3599 | N   | GLN | B | 172 | 48.536 | 46.660 | 73.377 | 1.00 | 22.79 |
| ATOM | 3600 | CA  | GLN | B | 172 | 47.630 | 47.237 | 74.358 | 1.00 | 37.17 |
| ATOM | 3601 | CB  | GLN | B | 172 | 47.376 | 48.734 | 74.126 | 1.00 | 40.40 |
| ATOM | 3602 | CG  | GLN | B | 172 | 46.844 | 49.424 | 75.378 | 1.00 | 50.87 |
| ATOM | 3603 | CD  | GLN | B | 172 | 46.684 | 50.924 | 75.272 | 1.00 | 51.56 |
| ATOM | 3604 | OE1 | GLN | B | 172 | 46.258 | 51.440 | 74.240 | 1.00 | 46.34 |
| ATOM | 3605 | NE2 | GLN | B | 172 | 47.013 | 51.651 | 76.339 | 1.00 | 33.78 |
| ATOM | 3606 | C   | GLN | B | 172 | 46.300 | 46.486 | 74.342 | 1.00 | 38.38 |
| ATOM | 3607 | O   | GLN | B | 172 | 45.611 | 46.417 | 73.322 | 1.00 | 24.25 |
| ATOM | 3608 | N   | MET | B | 173 | 45.967 | 45.927 | 75.511 | 1.00 | 30.63 |
| ATOM | 3609 | CA  | MET | B | 173 | 44.650 | 45.325 | 75.643 | 1.00 | 25.80 |
| ATOM | 3610 | CB  | MET | B | 173 | 44.534 | 44.392 | 76.853 | 1.00 | 20.42 |
| ATOM | 3611 | CG  | MET | B | 173 | 43.257 | 43.557 | 76.754 | 1.00 | 26.50 |
| ATOM | 3612 | SD  | MET | B | 173 | 43.176 | 42.237 | 77.997 | 1.00 | 36.50 |
| ATOM | 3613 | CE  | MET | B | 173 | 42.811 | 43.236 | 79.442 | 1.00 | 44.10 |
| ATOM | 3614 | C   | MET | B | 173 | 43.598 | 46.437 | 75.729 | 1.00 | 38.57 |
| ATOM | 3615 | O   | MET | B | 173 | 43.630 | 47.252 | 76.654 | 1.00 | 49.37 |
| ATOM | 3616 | N   | LEU | B | 174 | 42.707 | 46.443 | 74.754 | 1.00 | 32.34 |
| ATOM | 3617 | CA  | LEU | B | 174 | 41.663 | 47.434 | 74.587 | 1.00 | 32.40 |
| ATOM | 3618 | CB  | LEU | B | 174 | 41.355 | 47.609 | 73.093 | 1.00 | 27.63 |
| ATOM | 3619 | CG  | LEU | B | 174 | 41.749 | 48.955 | 72.490 | 1.00 | 42.29 |
| ATOM | 3620 | CD1 | LEU | B | 174 | 42.587 | 48.766 | 71.239 | 1.00 | 52.03 |
| ATOM | 3621 | CD2 | LEU | B | 174 | 40.490 | 49.769 | 72.215 | 1.00 | 46.08 |
| ATOM | 3622 | C   | LEU | B | 174 | 40.384 | 47.037 | 75.305 | 1.00 | 41.65 |
| ATOM | 3623 | O   | LEU | B | 174 | 39.616 | 47.862 | 75.795 | 1.00 | 43.69 |
| ATOM | 3624 | N   | SER | B | 175 | 40.165 | 45.721 | 75.328 | 1.00 | 28.31 |
| ATOM | 3625 | CA  | SER | B | 175 | 38.911 | 45.204 | 75.845 | 1.00 | 21.60 |
| ATOM | 3626 | CB  | SER | B | 175 | 37.807 | 45.343 | 74.801 | 1.00 | 21.97 |
| ATOM | 3627 | OG  | SER | B | 175 | 37.672 | 44.133 | 74.073 | 1.00 | 61.12 |
| ATOM | 3628 | C   | SER | B | 175 | 39.059 | 43.732 | 76.238 | 1.00 | 31.76 |
| ATOM | 3629 | O   | SER | B | 175 | 39.831 | 43.018 | 75.598 | 1.00 | 21.28 |
| ATOM | 3630 | N   | GLU | B | 176 | 38.305 | 43.370 | 77.266 | 1.00 | 32.04 |
| ATOM | 3631 | CA  | GLU | B | 176 | 38.286 | 42.031 | 77.838 | 1.00 | 33.85 |
| ATOM | 3632 | CB  | GLU | B | 176 | 39.330 | 41.927 | 78.969 | 1.00 | 27.59 |
| ATOM | 3633 | CG  | GLU | B | 176 | 39.308 | 40.570 | 79.654 | 1.00 | 29.03 |
| ATOM | 3634 | CD  | GLU | B | 176 | 40.283 | 40.373 | 80.782 | 1.00 | 40.65 |
| ATOM | 3635 | OE1 | GLU | B | 176 | 39.972 | 40.727 | 81.940 | 1.00 | 49.86 |
| ATOM | 3636 | OE2 | GLU | B | 176 | 41.389 | 39.838 | 80.534 | 1.00 | 40.12 |
| ATOM | 3637 | C   | GLU | B | 176 | 36.889 | 41.675 | 78.328 | 1.00 | 39.65 |
| ATOM | 3638 | O   | GLU | B | 176 | 36.400 | 42.226 | 79.318 | 1.00 | 44.09 |
| ATOM | 3639 | N   | SER | B | 177 | 36.195 | 40.757 | 77.654 | 1.00 | 38.39 |

**FIGURE 172**



Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 3640 | CA  | SER B 177 | 34.858 | 40.361 | 78.111 | 1.00 | 40.70 |
| ATOM | 3641 | CB  | SER B 177 | 33.787 | 40.649 | 77.069 | 1.00 | 44.75 |
| ATOM | 3642 | OG  | SER B 177 | 33.979 | 39.939 | 75.863 | 1.00 | 61.24 |
| ATOM | 3643 | C   | SER B 177 | 34.856 | 38.884 | 78.518 | 1.00 | 38.46 |
| ATOM | 3644 | O   | SER B 177 | 35.006 | 37.984 | 77.695 | 1.00 | 25.34 |
| ATOM | 3645 | N   | VAL B 178 | 34.692 | 38.696 | 79.815 | 1.00 | 35.33 |
| ATOM | 3646 | CA  | VAL B 178 | 34.780 | 37.440 | 80.534 | 1.00 | 44.36 |
| ATOM | 3647 | CB  | VAL B 178 | 35.355 | 37.668 | 81.947 | 1.00 | 47.13 |
| ATOM | 3648 | CG1 | VAL B 178 | 35.862 | 36.376 | 82.570 | 1.00 | 47.45 |
| ATOM | 3649 | CG2 | VAL B 178 | 36.477 | 38.698 | 81.898 | 1.00 | 51.70 |
| ATOM | 3650 | C   | VAL B 178 | 33.419 | 36.763 | 80.621 | 1.00 | 45.86 |
| ATOM | 3651 | O   | VAL B 178 | 32.512 | 37.204 | 81.327 | 1.00 | 51.44 |
| ATOM | 3652 | N   | LEU B 179 | 33.283 | 35.674 | 79.872 | 1.00 | 37.27 |
| ATOM | 3653 | CA  | LEU B 179 | 32.036 | 34.908 | 79.851 | 1.00 | 34.97 |
| ATOM | 3654 | CB  | LEU B 179 | 31.628 | 34.661 | 78.400 | 1.00 | 37.51 |
| ATOM | 3655 | CG  | LEU B 179 | 30.834 | 35.785 | 77.730 | 1.00 | 43.44 |
| ATOM | 3656 | CD1 | LEU B 179 | 31.470 | 37.140 | 77.989 | 1.00 | 54.18 |
| ATOM | 3657 | CD2 | LEU B 179 | 30.704 | 35.528 | 76.237 | 1.00 | 54.36 |
| ATOM | 3658 | C   | LEU B 179 | 32.193 | 33.620 | 80.645 | 1.00 | 34.28 |
| ATOM | 3659 | O   | LEU B 179 | 33.309 | 33.220 | 81.010 | 1.00 | 36.89 |
| ATOM | 3660 | N   | PRO B 180 | 31.101 | 32.937 | 80.970 | 1.00 | 45.49 |
| ATOM | 3661 | CA  | PRO B 180 | 31.209 | 31.705 | 81.756 | 1.00 | 42.82 |
| ATOM | 3662 | CB  | PRO B 180 | 29.774 | 31.148 | 81.733 | 1.00 | 47.75 |
| ATOM | 3663 | CG  | PRO B 180 | 28.932 | 32.376 | 81.617 | 1.00 | 51.41 |
| ATOM | 3664 | CD  | PRO B 180 | 29.695 | 33.258 | 80.665 | 1.00 | 53.24 |
| ATOM | 3665 | C   | PRO B 180 | 32.153 | 30.666 | 81.176 | 1.00 | 31.68 |
| ATOM | 3666 | O   | PRO B 180 | 32.821 | 29.985 | 81.963 | 1.00 | 42.99 |
| ATOM | 3667 | N   | GLU B 181 | 32.242 | 30.482 | 79.858 | 1.00 | 28.10 |
| ATOM | 3668 | CA  | GLU B 181 | 33.166 | 29.435 | 79.396 | 1.00 | 30.70 |
| ATOM | 3669 | CB  | GLU B 181 | 32.420 | 28.305 | 78.697 | 1.00 | 24.19 |
| ATOM | 3670 | CG  | GLU B 181 | 31.130 | 27.923 | 79.409 | 1.00 | 35.82 |
| ATOM | 3671 | CD  | GLU B 181 | 30.054 | 27.533 | 78.413 | 1.00 | 40.31 |
| ATOM | 3672 | OE1 | GLU B 181 | 29.358 | 28.440 | 77.912 | 1.00 | 49.12 |
| ATOM | 3673 | OE2 | GLU B 181 | 29.924 | 26.323 | 78.142 | 1.00 | 45.80 |
| ATOM | 3674 | C   | GLU B 181 | 34.229 | 29.976 | 78.447 | 1.00 | 33.02 |
| ATOM | 3675 | O   | GLU B 181 | 35.127 | 29.240 | 78.043 | 1.00 | 34.02 |
| ATOM | 3676 | N   | TRP B 182 | 34.139 | 31.254 | 78.085 | 1.00 | 26.28 |
| ATOM | 3677 | CA  | TRP B 182 | 35.215 | 31.807 | 77.263 | 1.00 | 25.54 |
| ATOM | 3678 | CB  | TRP B 182 | 35.049 | 31.542 | 75.780 | 1.00 | 25.17 |
| ATOM | 3679 | CG  | TRP B 182 | 33.799 | 31.961 | 75.090 | 1.00 | 23.98 |
| ATOM | 3680 | CD1 | TRP B 182 | 33.495 | 33.162 | 74.507 | 1.00 | 27.11 |
| ATOM | 3681 | NE1 | TRP B 182 | 32.228 | 33.126 | 73.975 | 1.00 | 26.38 |
| ATOM | 3682 | CE2 | TRP B 182 | 31.689 | 31.888 | 74.210 | 1.00 | 29.12 |
| ATOM | 3683 | CD2 | TRP B 182 | 32.649 | 31.127 | 74.905 | 1.00 | 25.63 |
| ATOM | 3684 | CE3 | TRP B 182 | 32.372 | 29.806 | 75.280 | 1.00 | 26.46 |
| ATOM | 3685 | CZ3 | TRP B 182 | 31.130 | 29.299 | 74.938 | 1.00 | 31.22 |
| ATOM | 3686 | CH2 | TRP B 182 | 30.191 | 30.079 | 74.244 | 1.00 | 33.39 |
| ATOM | 3687 | CZ2 | TRP B 182 | 30.441 | 31.371 | 73.869 | 1.00 | 31.20 |
| ATOM | 3688 | C   | TRP B 182 | 35.337 | 33.308 | 77.529 | 1.00 | 27.72 |
| ATOM | 3689 | O   | TRP B 182 | 34.418 | 33.935 | 78.055 | 1.00 | 30.24 |
| ATOM | 3690 | N   | THR B 183 | 36.493 | 33.818 | 77.150 | 1.00 | 24.75 |
| ATOM | 3691 | CA  | THR B 183 | 36.809 | 35.234 | 77.261 | 1.00 | 29.67 |

**FIGURE 173**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3692 | CB  | THR | B | 183 | 37.897 | 35.481 | 78.320 | 1.00 | 36.72 |
| ATOM | 3693 | OG1 | THR | B | 183 | 37.419 | 35.055 | 79.606 | 1.00 | 30.73 |
| ATOM | 3694 | CG2 | THR | B | 183 | 38.218 | 36.961 | 78.455 | 1.00 | 25.96 |
| ATOM | 3695 | C   | THR | B | 183 | 37.263 | 35.756 | 75.903 | 1.00 | 23.78 |
| ATOM | 3696 | O   | THR | B | 183 | 38.157 | 35.191 | 75.276 | 1.00 | 16.05 |
| ATOM | 3697 | N   | ILE | B | 184 | 36.649 | 36.838 | 75.455 | 1.00 | 21.97 |
| ATOM | 3698 | CA  | ILE | B | 184 | 37.110 | 37.497 | 74.227 | 1.00 | 26.63 |
| ATOM | 3699 | CB  | ILE | B | 184 | 35.918 | 37.735 | 73.288 | 1.00 | 30.23 |
| ATOM | 3700 | CG1 | ILE | B | 184 | 35.305 | 36.415 | 72.797 | 1.00 | 29.99 |
| ATOM | 3701 | CD1 | ILE | B | 184 | 33.881 | 36.539 | 72.305 | 1.00 | 36.01 |
| ATOM | 3702 | CG2 | ILE | B | 184 | 36.293 | 38.648 | 72.133 | 1.00 | 24.86 |
| ATOM | 3703 | C   | ILE | B | 184 | 37.843 | 38.782 | 74.573 | 1.00 | 26.33 |
| ATOM | 3704 | O   | ILE | B | 184 | 37.296 | 39.625 | 75.285 | 1.00 | 27.53 |
| ATOM | 3705 | N   | ARG | B | 185 | 39.072 | 38.936 | 74.095 | 1.00 | 21.56 |
| ATOM | 3706 | CA  | ARG | B | 185 | 39.876 | 40.127 | 74.341 | 1.00 | 21.72 |
| ATOM | 3707 | CB  | ARG | B | 185 | 41.151 | 39.785 | 75.111 | 1.00 | 18.90 |
| ATOM | 3708 | CG  | ARG | B | 185 | 40.884 | 39.061 | 76.431 | 1.00 | 20.33 |
| ATOM | 3709 | CD  | ARG | B | 185 | 42.207 | 38.540 | 76.980 | 1.00 | 31.19 |
| ATOM | 3710 | NE  | ARG | B | 185 | 42.119 | 38.235 | 78.404 | 1.00 | 29.95 |
| ATOM | 3711 | CZ  | ARG | B | 185 | 41.905 | 37.012 | 78.867 | 1.00 | 30.90 |
| ATOM | 3712 | NH1 | ARG | B | 185 | 41.770 | 36.026 | 77.993 | 1.00 | 28.15 |
| ATOM | 3713 | NH2 | ARG | B | 185 | 41.831 | 36.768 | 80.165 | 1.00 | 26.93 |
| ATOM | 3714 | C   | ARG | B | 185 | 40.246 | 40.824 | 73.038 | 1.00 | 24.49 |
| ATOM | 3715 | O   | ARG | B | 185 | 40.342 | 40.197 | 71.990 | 1.00 | 22.11 |
| ATOM | 3716 | N   | GLU | B | 186 | 40.440 | 42.137 | 73.098 | 1.00 | 23.85 |
| ATOM | 3717 | CA  | GLU | B | 186 | 40.858 | 42.852 | 71.895 | 1.00 | 23.99 |
| ATOM | 3718 | CB  | GLU | B | 186 | 39.831 | 43.906 | 71.499 | 1.00 | 32.77 |
| ATOM | 3719 | CG  | GLU | B | 186 | 38.961 | 43.556 | 70.303 | 1.00 | 49.41 |
| ATOM | 3720 | CD  | GLU | B | 186 | 38.376 | 44.815 | 69.677 | 1.00 | 57.85 |
| ATOM | 3721 | OE1 | GLU | B | 186 | 38.831 | 45.212 | 68.585 | 1.00 | 58.65 |
| ATOM | 3722 | OE2 | GLU | B | 186 | 37.465 | 45.405 | 70.295 | 1.00 | 46.66 |
| ATOM | 3723 | C   | GLU | B | 186 | 42.215 | 43.486 | 72.141 | 1.00 | 20.03 |
| ATOM | 3724 | O   | GLU | B | 186 | 42.426 | 44.138 | 73.165 | 1.00 | 28.24 |
| ATOM | 3725 | N   | PHE | B | 187 | 43.151 | 43.295 | 71.214 | 1.00 | 19.91 |
| ATOM | 3726 | CA  | PHE | B | 187 | 44.452 | 43.922 | 71.357 | 1.00 | 17.69 |
| ATOM | 3727 | CB  | PHE | B | 187 | 45.562 | 42.872 | 71.461 | 1.00 | 24.10 |
| ATOM | 3728 | CG  | PHE | B | 187 | 45.394 | 41.859 | 72.581 | 1.00 | 26.73 |
| ATOM | 3729 | CD1 | PHE | B | 187 | 45.114 | 40.535 | 72.294 | 1.00 | 32.91 |
| ATOM | 3730 | CE1 | PHE | B | 187 | 44.967 | 39.593 | 73.304 | 1.00 | 27.10 |
| ATOM | 3731 | CZ  | PHE | B | 187 | 45.089 | 39.989 | 74.620 | 1.00 | 21.98 |
| ATOM | 3732 | CE2 | PHE | B | 187 | 45.369 | 41.308 | 74.928 | 1.00 | 27.08 |
| ATOM | 3733 | CD2 | PHE | B | 187 | 45.539 | 42.233 | 73.907 | 1.00 | 28.39 |
| ATOM | 3734 | C   | PHE | B | 187 | 44.809 | 44.842 | 70.189 | 1.00 | 27.70 |
| ATOM | 3735 | O   | PHE | B | 187 | 44.560 | 44.562 | 69.019 | 1.00 | 24.34 |
| ATOM | 3736 | N   | LYS | B | 188 | 45.446 | 45.953 | 70.538 | 1.00 | 29.92 |
| ATOM | 3737 | CA  | LYS | B | 188 | 46.049 | 46.816 | 69.521 | 1.00 | 36.57 |
| ATOM | 3738 | CB  | LYS | B | 188 | 45.678 | 48.276 | 69.774 | 1.00 | 42.75 |
| ATOM | 3739 | CG  | LYS | B | 188 | 46.817 | 49.269 | 69.641 | 1.00 | 52.83 |
| ATOM | 3740 | CD  | LYS | B | 188 | 46.349 | 50.713 | 69.711 | 1.00 | 58.55 |
| ATOM | 3741 | CE  | LYS | B | 188 | 46.124 | 51.181 | 71.139 | 1.00 | 59.40 |
| ATOM | 3742 | NZ  | LYS | B | 188 | 47.298 | 50.947 | 72.026 | 1.00 | 34.15 |
| ATOM | 3743 | C   | LYS | B | 188 | 47.553 | 46.584 | 69.518 | 1.00 | 30.49 |

**FIGURE 174**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3744 | O   | LYS | B | 188 | 48.240 | 46.624 | 70.539 | 1.00 | 22.92  |
| ATOM | 3745 | N   | ILE | B | 189 | 48.136 | 46.304 | 68.350 | 1.00 | 24.79  |
| ATOM | 3746 | CA  | ILE | B | 189 | 49.581 | 46.144 | 68.310 | 1.00 | 26.54  |
| ATOM | 3747 | CB  | ILE | B | 189 | 49.992 | 44.714 | 67.933 | 1.00 | 29.28  |
| ATOM | 3748 | CG1 | ILE | B | 189 | 51.461 | 44.597 | 67.523 | 1.00 | 33.98  |
| ATOM | 3749 | CD1 | ILE | B | 189 | 51.848 | 43.205 | 67.067 | 1.00 | 52.63  |
| ATOM | 3750 | CG2 | ILE | B | 189 | 49.079 | 44.160 | 66.853 | 1.00 | 36.95  |
| ATOM | 3751 | C   | ILE | B | 189 | 50.175 | 47.152 | 67.321 | 1.00 | 26.97  |
| ATOM | 3752 | O   | ILE | B | 189 | 49.539 | 47.447 | 66.312 | 1.00 | 25.84  |
| ATOM | 3753 | N   | CYS | B | 190 | 51.344 | 47.657 | 67.659 | 1.00 | 32.86  |
| ATOM | 3754 | CA  | CYS | B | 190 | 52.103 | 48.607 | 66.874 | 1.00 | 31.79  |
| ATOM | 3755 | CB  | CYS | B | 190 | 52.243 | 49.961 | 67.577 | 1.00 | 35.55  |
| ATOM | 3756 | SG  | CYS | B | 190 | 50.732 | 50.549 | 68.369 | 1.00 | 48.07  |
| ATOM | 3757 | C   | CYS | B | 190 | 53.492 | 48.052 | 66.576 | 1.00 | 32.84  |
| ATOM | 3758 | O   | CYS | B | 190 | 54.208 | 47.629 | 67.478 | 1.00 | 29.87  |
| ATOM | 3759 | N   | GLY | B | 191 | 53.858 | 48.065 | 65.295 | 1.00 | 35.69  |
| ATOM | 3760 | CA  | GLY | B | 191 | 55.151 | 47.519 | 64.910 | 1.00 | 46.05  |
| ATOM | 3761 | C   | GLY | B | 191 | 55.917 | 48.502 | 64.045 | 1.00 | 51.49  |
| ATOM | 3762 | O   | GLY | B | 191 | 55.540 | 49.677 | 64.025 | 1.00 | 57.04  |
| ATOM | 3763 | N   | GLU | B | 192 | 56.944 | 48.025 | 63.353 | 1.00 | 53.82  |
| ATOM | 3764 | CA  | GLU | B | 192 | 57.794 | 48.872 | 62.522 | 1.00 | 71.96  |
| ATOM | 3765 | CB  | GLU | B | 192 | 58.741 | 48.013 | 61.681 | 1.00 | 79.49  |
| ATOM | 3766 | CG  | GLU | B | 192 | 60.088 | 48.655 | 61.399 | 1.00 | 83.42  |
| ATOM | 3767 | CD  | GLU | B | 192 | 61.126 | 48.395 | 62.472 | 1.00 | 90.04  |
| ATOM | 3768 | OE1 | GLU | B | 192 | 60.759 | 48.211 | 63.654 | 1.00 | 98.44  |
| ATOM | 3769 | OE2 | GLU | B | 192 | 62.329 | 48.371 | 62.130 | 1.00 | 89.90  |
| ATOM | 3770 | C   | GLU | B | 192 | 56.969 | 49.797 | 61.622 | 1.00 | 79.73  |
| ATOM | 3771 | O   | GLU | B | 192 | 57.359 | 50.943 | 61.396 | 1.00 | 81.84  |
| ATOM | 3772 | N   | GLU | B | 193 | 55.861 | 49.274 | 61.154 | 1.00 | 88.39  |
| ATOM | 3773 | CA  | GLU | B | 193 | 54.815 | 49.806 | 60.317 | 1.00 | 96.64  |
| ATOM | 3774 | CB  | GLU | B | 193 | 54.932 | 51.307 | 60.055 | 1.00 | 98.26  |
| ATOM | 3775 | CG  | GLU | B | 193 | 53.693 | 51.905 | 59.401 | 1.00 | 98.54  |
| ATOM | 3776 | CD  | GLU | B | 193 | 53.567 | 53.404 | 59.562 | 1.00 | 97.01  |
| ATOM | 3777 | OE1 | GLU | B | 193 | 52.688 | 53.853 | 60.336 | 1.00 | 83.43  |
| ATOM | 3778 | OE2 | GLU | B | 193 | 54.330 | 54.154 | 58.911 | 1.00 | 98.66  |
| ATOM | 3779 | C   | GLU | B | 193 | 54.823 | 49.030 | 58.991 | 1.00 | 102.76 |
| ATOM | 3780 | O   | GLU | B | 193 | 54.656 | 49.612 | 57.926 | 1.00 | 116.30 |
| ATOM | 3781 | N   | GLN | B | 194 | 55.029 | 47.726 | 59.137 | 1.00 | 102.86 |
| ATOM | 3782 | CA  | GLN | B | 194 | 55.067 | 46.786 | 58.022 | 1.00 | 100.17 |
| ATOM | 3783 | CB  | GLN | B | 194 | 55.150 | 45.351 | 58.544 | 1.00 | 94.78  |
| ATOM | 3784 | CG  | GLN | B | 194 | 56.548 | 44.913 | 58.944 | 1.00 | 90.58  |
| ATOM | 3785 | CD  | GLN | B | 194 | 57.076 | 45.627 | 60.173 | 1.00 | 89.36  |
| ATOM | 3786 | OE1 | GLN | B | 194 | 56.393 | 46.444 | 60.792 | 1.00 | 75.86  |
| ATOM | 3787 | NE2 | GLN | B | 194 | 58.314 | 45.317 | 60.547 | 1.00 | 97.42  |
| ATOM | 3788 | C   | GLN | B | 194 | 53.848 | 46.979 | 57.135 | 1.00 | 100.06 |
| ATOM | 3789 | O   | GLN | B | 194 | 53.618 | 48.060 | 56.588 | 1.00 | 106.59 |
| ATOM | 3790 | N   | LEU | B | 195 | 53.019 | 45.946 | 56.971 | 1.00 | 96.75  |
| ATOM | 3791 | CA  | LEU | B | 195 | 51.800 | 46.199 | 56.191 | 1.00 | 92.05  |
| ATOM | 3792 | CB  | LEU | B | 195 | 51.420 | 44.991 | 55.342 | 1.00 | 85.63  |
| ATOM | 3793 | CG  | LEU | B | 195 | 51.792 | 45.085 | 53.856 | 1.00 | 78.28  |
| ATOM | 3794 | CD1 | LEU | B | 195 | 53.216 | 44.593 | 53.634 | 1.00 | 84.54  |
| ATOM | 3795 | CD2 | LEU | B | 195 | 50.811 | 44.310 | 52.989 | 1.00 | 43.11  |

**FIGURE 175**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |        |        |      |        |
|------|------|-----|-----------|--------|--------|--------|------|--------|
| ATOM | 3796 | C   | LEU B 195 | 50.684 | 46.623 | 57.141 | 1.00 | 93.25  |
| ATOM | 3797 | O   | LEU B 195 | 49.499 | 46.559 | 56.823 | 1.00 | 106.23 |
| ATOM | 3798 | N   | ASP B 196 | 51.100 | 47.071 | 58.323 | 1.00 | 88.54  |
| ATOM | 3799 | CA  | ASP B 196 | 50.208 | 47.654 | 59.311 | 1.00 | 85.36  |
| ATOM | 3800 | CB  | ASP B 196 | 49.937 | 46.706 | 60.472 | 1.00 | 77.13  |
| ATOM | 3801 | CG  | ASP B 196 | 50.263 | 45.256 | 60.196 | 1.00 | 69.71  |
| ATOM | 3802 | OD1 | ASP B 196 | 51.435 | 44.924 | 59.922 | 1.00 | 56.81  |
| ATOM | 3803 | OD2 | ASP B 196 | 49.318 | 44.442 | 60.267 | 1.00 | 49.34  |
| ATOM | 3804 | C   | ASP B 196 | 50.795 | 48.962 | 59.853 | 1.00 | 86.61  |
| ATOM | 3805 | O   | ASP B 196 | 52.000 | 49.194 | 59.771 | 1.00 | 72.64  |
| ATOM | 3806 | N   | ALA B 197 | 49.924 | 49.797 | 60.398 | 1.00 | 87.67  |
| ATOM | 3807 | CA  | ALA B 197 | 50.287 | 51.051 | 61.042 | 1.00 | 89.69  |
| ATOM | 3808 | CB  | ALA B 197 | 50.135 | 52.222 | 60.096 | 1.00 | 83.48  |
| ATOM | 3809 | C   | ALA B 197 | 49.426 | 51.223 | 62.302 | 1.00 | 94.67  |
| ATOM | 3810 | O   | ALA B 197 | 49.317 | 52.318 | 62.843 | 1.00 | 100.04 |
| ATOM | 3811 | N   | HIS B 198 | 48.864 | 50.096 | 62.692 | 1.00 | 93.88  |
| ATOM | 3812 | CA  | HIS B 198 | 47.955 | 49.838 | 63.785 | 1.00 | 88.36  |
| ATOM | 3813 | CB  | HIS B 198 | 47.173 | 51.099 | 64.161 | 1.00 | 92.99  |
| ATOM | 3814 | CG  | HIS B 198 | 45.965 | 50.823 | 64.998 | 1.00 | 104.14 |
| ATOM | 3815 | ND1 | HIS B 198 | 46.045 | 50.478 | 66.329 | 1.00 | 108.50 |
| ATOM | 3816 | CE1 | HIS B 198 | 44.830 | 50.292 | 66.813 | 1.00 | 111.40 |
| ATOM | 3817 | NE2 | HIS B 198 | 43.960 | 50.506 | 65.840 | 1.00 | 112.45 |
| ATOM | 3818 | CD2 | HIS B 198 | 44.647 | 50.839 | 64.696 | 1.00 | 109.03 |
| ATOM | 3819 | C   | HIS B 198 | 46.988 | 48.711 | 63.416 | 1.00 | 81.60  |
| ATOM | 3820 | O   | HIS B 198 | 46.100 | 48.902 | 62.581 | 1.00 | 85.74  |
| ATOM | 3821 | N   | ARG B 199 | 47.151 | 47.537 | 64.020 | 1.00 | 68.93  |
| ATOM | 3822 | CA  | ARG B 199 | 46.278 | 46.398 | 63.754 | 1.00 | 51.46  |
| ATOM | 3823 | CB  | ARG B 199 | 47.089 | 45.192 | 63.265 | 1.00 | 49.03  |
| ATOM | 3824 | CG  | ARG B 199 | 46.204 | 44.080 | 62.716 | 1.00 | 46.46  |
| ATOM | 3825 | CD  | ARG B 199 | 46.953 | 42.775 | 62.585 | 1.00 | 51.43  |
| ATOM | 3826 | NE  | ARG B 199 | 48.202 | 42.873 | 61.850 | 1.00 | 58.26  |
| ATOM | 3827 | CZ  | ARG B 199 | 49.185 | 41.980 | 61.891 | 1.00 | 57.04  |
| ATOM | 3828 | NH1 | ARG B 199 | 49.068 | 40.896 | 62.649 | 1.00 | 28.91  |
| ATOM | 3829 | NH2 | ARG B 199 | 50.288 | 42.168 | 61.174 | 1.00 | 39.20  |
| ATOM | 3830 | C   | ARG B 199 | 45.464 | 46.004 | 64.987 | 1.00 | 33.01  |
| ATOM | 3831 | O   | ARG B 199 | 45.928 | 46.200 | 66.112 | 1.00 | 29.63  |
| ATOM | 3832 | N   | LEU B 200 | 44.268 | 45.459 | 64.781 | 1.00 | 24.89  |
| ATOM | 3833 | CA  | LEU B 200 | 43.422 | 45.004 | 65.880 | 1.00 | 27.88  |
| ATOM | 3834 | CB  | LEU B 200 | 42.010 | 45.570 | 65.783 | 1.00 | 34.27  |
| ATOM | 3835 | CG  | LEU B 200 | 41.523 | 46.288 | 67.047 | 1.00 | 42.11  |
| ATOM | 3836 | CD1 | LEU B 200 | 41.605 | 45.366 | 68.249 | 1.00 | 45.77  |
| ATOM | 3837 | CD2 | LEU B 200 | 42.333 | 47.553 | 67.292 | 1.00 | 51.38  |
| ATOM | 3838 | C   | LEU B 200 | 43.353 | 43.477 | 65.913 | 1.00 | 30.00  |
| ATOM | 3839 | O   | LEU B 200 | 42.871 | 42.868 | 64.959 | 1.00 | 32.82  |
| ATOM | 3840 | N   | ILE B 201 | 43.834 | 42.882 | 67.003 | 1.00 | 28.87  |
| ATOM | 3841 | CA  | ILE B 201 | 43.821 | 41.425 | 67.118 | 1.00 | 24.18  |
| ATOM | 3842 | CB  | ILE B 201 | 45.174 | 40.900 | 67.623 | 1.00 | 24.29  |
| ATOM | 3843 | CG1 | ILE B 201 | 46.350 | 41.222 | 66.696 | 1.00 | 28.49  |
| ATOM | 3844 | CD1 | ILE B 201 | 45.941 | 41.124 | 65.247 | 1.00 | 39.78  |
| ATOM | 3845 | CG2 | ILE B 201 | 45.105 | 39.401 | 67.873 | 1.00 | 25.71  |
| ATOM | 3846 | C   | ILE B 201 | 42.717 | 40.972 | 68.059 | 1.00 | 22.16  |
| ATOM | 3847 | O   | ILE B 201 | 42.640 | 41.494 | 69.168 | 1.00 | 23.92  |

**FIGURE 176**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 3848 | N   | ARG | B | 202 | 41.883 | 40.037 | 67.647 | 1.00 | 18.44 |
| ATOM | 3849 | CA  | ARG | B | 202 | 40.849 | 39.447 | 68.478 | 1.00 | 22.50 |
| ATOM | 3850 | CB  | ARG | B | 202 | 39.585 | 39.119 | 67.693 | 1.00 | 33.06 |
| ATOM | 3851 | CG  | ARG | B | 202 | 38.305 | 39.726 | 68.233 | 1.00 | 52.62 |
| ATOM | 3852 | CD  | ARG | B | 202 | 37.344 | 40.048 | 67.098 | 1.00 | 66.81 |
| ATOM | 3853 | NE  | ARG | B | 202 | 36.728 | 41.358 | 67.260 | 1.00 | 75.75 |
| ATOM | 3854 | CZ  | ARG | B | 202 | 37.372 | 42.512 | 67.362 | 1.00 | 85.03 |
| ATOM | 3855 | NH1 | ARG | B | 202 | 38.698 | 42.553 | 67.322 | 1.00 | 98.51 |
| ATOM | 3856 | NH2 | ARG | B | 202 | 36.677 | 43.635 | 67.506 | 1.00 | 92.03 |
| ATOM | 3857 | C   | ARG | B | 202 | 41.359 | 38.141 | 69.099 | 1.00 | 26.96 |
| ATOM | 3858 | O   | ARG | B | 202 | 41.955 | 37.319 | 68.410 | 1.00 | 18.58 |
| ATOM | 3859 | N   | HIS | B | 203 | 41.120 | 37.977 | 70.384 | 1.00 | 28.22 |
| ATOM | 3860 | CA  | HIS | B | 203 | 41.595 | 36.823 | 71.148 | 1.00 | 23.47 |
| ATOM | 3861 | CB  | HIS | B | 203 | 42.637 | 37.287 | 72.150 | 1.00 | 18.39 |
| ATOM | 3862 | CG  | HIS | B | 203 | 43.392 | 36.213 | 72.850 | 1.00 | 20.01 |
| ATOM | 3863 | ND1 | HIS | B | 203 | 42.935 | 35.618 | 73.999 | 1.00 | 22.68 |
| ATOM | 3864 | CE1 | HIS | B | 203 | 43.797 | 34.707 | 74.400 | 1.00 | 22.72 |
| ATOM | 3865 | NE2 | HIS | B | 203 | 44.809 | 34.694 | 73.548 | 1.00 | 18.58 |
| ATOM | 3866 | CD2 | HIS | B | 203 | 44.580 | 35.624 | 72.563 | 1.00 | 22.68 |
| ATOM | 3867 | C   | HIS | B | 203 | 40.398 | 36.148 | 71.813 | 1.00 | 23.95 |
| ATOM | 3868 | O   | HIS | B | 203 | 39.651 | 36.785 | 72.562 | 1.00 | 18.73 |
| ATOM | 3869 | N   | PHE | B | 204 | 40.248 | 34.876 | 71.479 | 1.00 | 17.03 |
| ATOM | 3870 | CA  | PHE | B | 204 | 39.161 | 33.994 | 71.840 | 1.00 | 16.70 |
| ATOM | 3871 | CB  | PHE | B | 204 | 38.534 | 33.311 | 70.614 | 1.00 | 22.28 |
| ATOM | 3872 | CG  | PHE | B | 204 | 38.026 | 34.329 | 69.604 | 1.00 | 24.33 |
| ATOM | 3873 | CD1 | PHE | B | 204 | 38.876 | 34.813 | 68.622 | 1.00 | 22.40 |
| ATOM | 3874 | CE1 | PHE | B | 204 | 38.411 | 35.764 | 67.735 | 1.00 | 18.80 |
| ATOM | 3875 | CZ  | PHE | B | 204 | 37.103 | 36.205 | 67.847 | 1.00 | 19.32 |
| ATOM | 3876 | CE2 | PHE | B | 204 | 36.244 | 35.727 | 68.811 | 1.00 | 25.22 |
| ATOM | 3877 | CD2 | PHE | B | 204 | 36.716 | 34.768 | 69.694 | 1.00 | 26.02 |
| ATOM | 3878 | C   | PHE | B | 204 | 39.702 | 32.924 | 72.788 | 1.00 | 22.01 |
| ATOM | 3879 | O   | PHE | B | 204 | 40.366 | 31.995 | 72.324 | 1.00 | 24.15 |
| ATOM | 3880 | N   | HIS | B | 205 | 39.416 | 33.083 | 74.068 | 1.00 | 17.87 |
| ATOM | 3881 | CA  | HIS | B | 205 | 40.000 | 32.212 | 75.077 | 1.00 | 18.30 |
| ATOM | 3882 | CB  | HIS | B | 205 | 40.620 | 33.068 | 76.193 | 1.00 | 17.58 |
| ATOM | 3883 | CG  | HIS | B | 205 | 41.469 | 32.282 | 77.137 | 1.00 | 20.30 |
| ATOM | 3884 | ND1 | HIS | B | 205 | 41.954 | 32.812 | 78.310 | 1.00 | 22.02 |
| ATOM | 3885 | CE1 | HIS | B | 205 | 42.670 | 31.902 | 78.946 | 1.00 | 21.93 |
| ATOM | 3886 | NE2 | HIS | B | 205 | 42.663 | 30.786 | 78.227 | 1.00 | 22.68 |
| ATOM | 3887 | CD2 | HIS | B | 205 | 41.915 | 31.001 | 77.092 | 1.00 | 15.40 |
| ATOM | 3888 | C   | HIS | B | 205 | 38.958 | 31.270 | 75.658 | 1.00 | 23.56 |
| ATOM | 3889 | O   | HIS | B | 205 | 38.102 | 31.697 | 76.438 | 1.00 | 19.47 |
| ATOM | 3890 | N   | TYR | B | 206 | 39.032 | 29.996 | 75.287 | 1.00 | 18.88 |
| ATOM | 3891 | CA  | TYR | B | 206 | 38.073 | 29.022 | 75.836 | 1.00 | 22.05 |
| ATOM | 3892 | CB  | TYR | B | 206 | 37.855 | 27.895 | 74.846 | 1.00 | 20.72 |
| ATOM | 3893 | CG  | TYR | B | 206 | 36.757 | 26.923 | 75.209 | 1.00 | 18.73 |
| ATOM | 3894 | CD1 | TYR | B | 206 | 35.420 | 27.266 | 75.039 | 1.00 | 20.87 |
| ATOM | 3895 | CE1 | TYR | B | 206 | 34.413 | 26.376 | 75.372 | 1.00 | 26.51 |
| ATOM | 3896 | CZ  | TYR | B | 206 | 34.752 | 25.135 | 75.870 | 1.00 | 28.96 |
| ATOM | 3897 | OH  | TYR | B | 206 | 33.753 | 24.244 | 76.205 | 1.00 | 33.83 |
| ATOM | 3898 | CE2 | TYR | B | 206 | 36.067 | 24.773 | 76.049 | 1.00 | 30.27 |
| ATOM | 3899 | CD2 | TYR | B | 206 | 37.073 | 25.671 | 75.719 | 1.00 | 28.39 |

**FIGURE 177**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |       |        |        |        |      |       |
|------|------|-----|-----|-------|--------|--------|--------|------|-------|
| ATOM | 3900 | C   | TYR | B 206 | 38.613 | 28.499 | 77.156 | 1.00 | 24.76 |
| ATOM | 3901 | O   | TYR | B 206 | 39.717 | 27.943 | 77.181 | 1.00 | 19.80 |
| ATOM | 3902 | N   | THR | B 207 | 37.887 | 28.679 | 78.261 | 1.00 | 20.66 |
| ATOM | 3903 | CA  | THR | B 207 | 38.554 | 28.426 | 79.533 | 1.00 | 20.59 |
| ATOM | 3904 | CB  | THR | B 207 | 38.343 | 29.630 | 80.477 | 1.00 | 23.62 |
| ATOM | 3905 | OG1 | THR | B 207 | 36.964 | 30.008 | 80.399 | 1.00 | 20.08 |
| ATOM | 3906 | CG2 | THR | B 207 | 39.198 | 30.803 | 80.014 | 1.00 | 30.98 |
| ATOM | 3907 | C   | THR | B 207 | 38.084 | 27.179 | 80.263 | 1.00 | 23.84 |
| ATOM | 3908 | O   | THR | B 207 | 38.498 | 26.972 | 81.414 | 1.00 | 22.22 |
| ATOM | 3909 | N   | VAL | B 208 | 37.254 | 26.345 | 79.643 | 1.00 | 23.82 |
| ATOM | 3910 | CA  | VAL | B 208 | 36.825 | 25.167 | 80.402 | 1.00 | 28.06 |
| ATOM | 3911 | CB  | VAL | B 208 | 35.322 | 25.266 | 80.749 | 1.00 | 27.30 |
| ATOM | 3912 | CG1 | VAL | B 208 | 35.074 | 26.517 | 81.590 | 1.00 | 32.43 |
| ATOM | 3913 | CG2 | VAL | B 208 | 34.465 | 25.241 | 79.494 | 1.00 | 27.40 |
| ATOM | 3914 | C   | VAL | B 208 | 37.116 | 23.851 | 79.698 | 1.00 | 30.84 |
| ATOM | 3915 | O   | VAL | B 208 | 36.320 | 22.909 | 79.773 | 1.00 | 35.95 |
| ATOM | 3916 | N   | TRP | B 209 | 38.255 | 23.743 | 79.031 | 1.00 | 26.26 |
| ATOM | 3917 | CA  | TRP | B 209 | 38.657 | 22.486 | 78.391 | 1.00 | 24.69 |
| ATOM | 3918 | CB  | TRP | B 209 | 38.976 | 22.685 | 76.918 | 1.00 | 30.19 |
| ATOM | 3919 | CG  | TRP | B 209 | 39.163 | 21.465 | 76.068 | 1.00 | 24.30 |
| ATOM | 3920 | CD1 | TRP | B 209 | 39.449 | 20.169 | 76.361 | 1.00 | 26.73 |
| ATOM | 3921 | NE1 | TRP | B 209 | 39.526 | 19.394 | 75.229 | 1.00 | 27.16 |
| ATOM | 3922 | CE2 | TRP | B 209 | 39.278 | 20.210 | 74.148 | 1.00 | 34.57 |
| ATOM | 3923 | CD2 | TRP | B 209 | 39.048 | 21.513 | 74.632 | 1.00 | 23.58 |
| ATOM | 3924 | CE3 | TRP | B 209 | 38.768 | 22.558 | 73.746 | 1.00 | 24.70 |
| ATOM | 3925 | CZ3 | TRP | B 209 | 38.731 | 22.256 | 72.395 | 1.00 | 35.51 |
| ATOM | 3926 | CH2 | TRP | B 209 | 38.964 | 20.951 | 71.930 | 1.00 | 33.08 |
| ATOM | 3927 | CZ2 | TRP | B 209 | 39.236 | 19.917 | 72.782 | 1.00 | 32.65 |
| ATOM | 3928 | C   | TRP | B 209 | 39.889 | 21.934 | 79.099 | 1.00 | 26.90 |
| ATOM | 3929 | O   | TRP | B 209 | 40.981 | 22.462 | 78.880 | 1.00 | 24.25 |
| ATOM | 3930 | N   | PRO | B 210 | 39.733 | 20.881 | 79.886 | 1.00 | 30.43 |
| ATOM | 3931 | CA  | PRO | B 210 | 40.872 | 20.308 | 80.611 | 1.00 | 22.74 |
| ATOM | 3932 | CB  | PRO | B 210 | 40.241 | 19.228 | 81.492 | 1.00 | 26.14 |
| ATOM | 3933 | CG  | PRO | B 210 | 38.776 | 19.517 | 81.488 | 1.00 | 31.27 |
| ATOM | 3934 | CD  | PRO | B 210 | 38.486 | 20.136 | 80.147 | 1.00 | 27.01 |
| ATOM | 3935 | C   | PRO | B 210 | 41.871 | 19.648 | 79.668 | 1.00 | 22.10 |
| ATOM | 3936 | O   | PRO | B 210 | 41.475 | 19.064 | 78.662 | 1.00 | 34.64 |
| ATOM | 3937 | N   | ASP | B 211 | 43.153 | 19.724 | 80.001 | 1.00 | 15.18 |
| ATOM | 3938 | CA  | ASP | B 211 | 44.183 | 19.090 | 79.209 | 1.00 | 21.45 |
| ATOM | 3939 | CB  | ASP | B 211 | 45.565 | 19.247 | 79.849 | 1.00 | 28.68 |
| ATOM | 3940 | CG  | ASP | B 211 | 46.648 | 19.134 | 78.790 | 1.00 | 26.69 |
| ATOM | 3941 | OD1 | ASP | B 211 | 47.820 | 19.370 | 79.138 | 1.00 | 34.33 |
| ATOM | 3942 | OD2 | ASP | B 211 | 46.281 | 18.819 | 77.638 | 1.00 | 25.77 |
| ATOM | 3943 | C   | ASP | B 211 | 43.901 | 17.600 | 79.038 | 1.00 | 40.98 |
| ATOM | 3944 | O   | ASP | B 211 | 43.349 | 16.940 | 79.926 | 1.00 | 28.43 |
| ATOM | 3945 | N   | HIS | B 212 | 44.254 | 17.081 | 77.868 | 1.00 | 34.69 |
| ATOM | 3946 | CA  | HIS | B 212 | 44.020 | 15.705 | 77.459 | 1.00 | 29.07 |
| ATOM | 3947 | CB  | HIS | B 212 | 44.864 | 14.770 | 78.328 | 1.00 | 22.05 |
| ATOM | 3948 | CG  | HIS | B 212 | 46.266 | 15.247 | 78.527 | 1.00 | 23.98 |
| ATOM | 3949 | ND1 | HIS | B 212 | 47.183 | 15.323 | 77.504 | 1.00 | 29.39 |
| ATOM | 3950 | CE1 | HIS | B 212 | 48.329 | 15.777 | 77.969 | 1.00 | 33.66 |
| ATOM | 3951 | NE2 | HIS | B 212 | 48.187 | 15.996 | 79.268 | 1.00 | 32.42 |

**FIGURE 178**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 3952 | CD2 | HIS | B | 212 | 46.906 | 15.670 | 79.637 | 1.00 | 23.94  |
| ATOM | 3953 | C   | HIS | B | 212 | 42.564 | 15.267 | 77.538 | 1.00 | 39.31  |
| ATOM | 3954 | O   | HIS | B | 212 | 42.251 | 14.074 | 77.466 | 1.00 | 50.27  |
| ATOM | 3955 | N   | GLY | B | 213 | 41.642 | 16.207 | 77.683 | 1.00 | 40.41  |
| ATOM | 3956 | CA  | GLY | B | 213 | 40.245 | 15.925 | 77.912 | 1.00 | 30.96  |
| ATOM | 3957 | C   | GLY | B | 213 | 39.401 | 16.580 | 76.835 | 1.00 | 33.95  |
| ATOM | 3958 | O   | GLY | B | 213 | 39.938 | 17.004 | 75.817 | 1.00 | 33.78  |
| ATOM | 3959 | N   | VAL | B | 214 | 38.120 | 16.610 | 77.144 | 1.00 | 31.79  |
| ATOM | 3960 | CA  | VAL | B | 214 | 37.081 | 17.170 | 76.303 | 1.00 | 31.65  |
| ATOM | 3961 | CB  | VAL | B | 214 | 36.238 | 16.035 | 75.701 | 1.00 | 35.28  |
| ATOM | 3962 | CG1 | VAL | B | 214 | 37.120 | 15.151 | 74.832 | 1.00 | 45.38  |
| ATOM | 3963 | CG2 | VAL | B | 214 | 35.582 | 15.230 | 76.815 | 1.00 | 24.44  |
| ATOM | 3964 | C   | VAL | B | 214 | 36.205 | 18.070 | 77.150 | 1.00 | 36.18  |
| ATOM | 3965 | O   | VAL | B | 214 | 36.097 | 17.826 | 78.358 | 1.00 | 35.44  |
| ATOM | 3966 | N   | PRO | B | 215 | 35.582 | 19.094 | 76.597 | 1.00 | 32.79  |
| ATOM | 3967 | CA  | PRO | B | 215 | 34.679 | 19.888 | 77.449 | 1.00 | 35.01  |
| ATOM | 3968 | CB  | PRO | B | 215 | 34.113 | 20.923 | 76.488 | 1.00 | 32.92  |
| ATOM | 3969 | CG  | PRO | B | 215 | 35.146 | 21.018 | 75.406 | 1.00 | 39.93  |
| ATOM | 3970 | CD  | PRO | B | 215 | 35.654 | 19.604 | 75.225 | 1.00 | 33.73  |
| ATOM | 3971 | C   | PRO | B | 215 | 33.574 | 18.999 | 78.031 | 1.00 | 40.15  |
| ATOM | 3972 | O   | PRO | B | 215 | 33.366 | 17.872 | 77.581 | 1.00 | 31.33  |
| ATOM | 3973 | N   | GLU | B | 216 | 32.896 | 19.532 | 79.028 | 1.00 | 39.88  |
| ATOM | 3974 | CA  | GLU | B | 216 | 31.810 | 18.913 | 79.763 | 1.00 | 43.51  |
| ATOM | 3975 | CB  | GLU | B | 216 | 31.406 | 19.850 | 80.906 | 1.00 | 52.27  |
| ATOM | 3976 | CG  | GLU | B | 216 | 31.040 | 19.159 | 82.203 | 1.00 | 67.80  |
| ATOM | 3977 | CD  | GLU | B | 216 | 31.677 | 19.781 | 83.429 | 1.00 | 77.24  |
| ATOM | 3978 | OE1 | GLU | B | 216 | 31.550 | 19.193 | 84.527 | 1.00 | 81.69  |
| ATOM | 3979 | OE2 | GLU | B | 216 | 32.302 | 20.857 | 83.300 | 1.00 | 89.24  |
| ATOM | 3980 | C   | GLU | B | 216 | 30.617 | 18.606 | 78.864 | 1.00 | 40.84  |
| ATOM | 3981 | O   | GLU | B | 216 | 30.010 | 17.536 | 78.967 | 1.00 | 53.80  |
| ATOM | 3982 | N   | THR | B | 217 | 30.269 | 19.531 | 77.983 | 1.00 | 38.95  |
| ATOM | 3983 | CA  | THR | B | 217 | 29.204 | 19.383 | 77.008 | 1.00 | 42.02  |
| ATOM | 3984 | CB  | THR | B | 217 | 28.040 | 20.379 | 77.205 | 1.00 | 45.29  |
| ATOM | 3985 | OG1 | THR | B | 217 | 28.483 | 21.708 | 76.887 | 1.00 | 35.12  |
| ATOM | 3986 | CG2 | THR | B | 217 | 27.573 | 20.406 | 78.649 | 1.00 | 41.50  |
| ATOM | 3987 | C   | THR | B | 217 | 29.708 | 19.600 | 75.580 | 1.00 | 41.46  |
| ATOM | 3988 | O   | THR | B | 217 | 30.806 | 20.088 | 75.328 | 1.00 | 31.75  |
| ATOM | 3989 | N   | THR | B | 218 | 28.852 | 19.241 | 74.631 | 1.00 | 44.21  |
| ATOM | 3990 | CA  | THR | B | 218 | 29.157 | 19.469 | 73.222 | 1.00 | 46.58  |
| ATOM | 3991 | CB  | THR | B | 218 | 28.428 | 18.436 | 72.347 | 1.00 | 50.20  |
| ATOM | 3992 | OG1 | THR | B | 218 | 27.030 | 18.755 | 72.322 | 1.00 | 60.14  |
| ATOM | 3993 | CG2 | THR | B | 218 | 28.539 | 17.047 | 72.953 | 1.00 | 48.45  |
| ATOM | 3994 | C   | THR | B | 218 | 28.751 | 20.877 | 72.807 | 1.00 | 39.87  |
| ATOM | 3995 | O   | THR | B | 218 | 29.472 | 21.575 | 72.100 | 1.00 | 33.12  |
| ATOM | 3996 | N   | GLN | B | 219 | 27.581 | 21.301 | 73.262 | 1.00 | 42.47  |
| ATOM | 3997 | CA  | GLN | B | 219 | 27.023 | 22.603 | 72.942 | 1.00 | 48.42  |
| ATOM | 3998 | CB  | GLN | B | 219 | 25.735 | 22.859 | 73.734 | 1.00 | 61.04  |
| ATOM | 3999 | CG  | GLN | B | 219 | 24.465 | 22.396 | 73.043 | 1.00 | 75.20  |
| ATOM | 4000 | CD  | GLN | B | 219 | 23.709 | 21.356 | 73.846 | 1.00 | 86.54  |
| ATOM | 4001 | OE1 | GLN | B | 219 | 24.156 | 20.217 | 73.990 | 1.00 | 100.39 |
| ATOM | 4002 | NE2 | GLN | B | 219 | 22.552 | 21.750 | 74.373 | 1.00 | 96.05  |
| ATOM | 4003 | C   | GLN | B | 219 | 27.988 | 23.745 | 73.241 | 1.00 | 42.13  |

**FIGURE 179**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 4004 | O   | GLN B 219 | 27.912 | 24.784 | 72.588 | 1.00 | 38.02 |
| ATOM | 4005 | N   | SER B 220 | 28.856 | 23.557 | 74.230 | 1.00 | 41.58 |
| ATOM | 4006 | CA  | SER B 220 | 29.702 | 24.652 | 74.687 | 1.00 | 41.47 |
| ATOM | 4007 | CB  | SER B 220 | 30.377 | 24.324 | 76.022 | 1.00 | 40.77 |
| ATOM | 4008 | OG  | SER B 220 | 31.170 | 25.425 | 76.432 | 1.00 | 52.01 |
| ATOM | 4009 | C   | SER B 220 | 30.781 | 24.985 | 73.661 | 1.00 | 32.19 |
| ATOM | 4010 | O   | SER B 220 | 30.948 | 26.137 | 73.270 | 1.00 | 34.50 |
| ATOM | 4011 | N   | LEU B 221 | 31.491 | 23.939 | 73.262 | 1.00 | 32.63 |
| ATOM | 4012 | CA  | LEU B 221 | 32.578 | 24.130 | 72.312 | 1.00 | 30.11 |
| ATOM | 4013 | CB  | LEU B 221 | 33.532 | 22.934 | 72.268 | 1.00 | 31.66 |
| ATOM | 4014 | CG  | LEU B 221 | 34.848 | 23.244 | 71.525 | 1.00 | 33.07 |
| ATOM | 4015 | CD1 | LEU B 221 | 35.653 | 24.288 | 72.290 | 1.00 | 29.11 |
| ATOM | 4016 | CD2 | LEU B 221 | 35.641 | 21.978 | 71.284 | 1.00 | 29.80 |
| ATOM | 4017 | C   | LEU B 221 | 31.970 | 24.416 | 70.944 | 1.00 | 30.52 |
| ATOM | 4018 | O   | LEU B 221 | 32.479 | 25.263 | 70.210 | 1.00 | 31.28 |
| ATOM | 4019 | N   | ILE B 222 | 30.879 | 23.712 | 70.649 | 1.00 | 30.64 |
| ATOM | 4020 | CA  | ILE B 222 | 30.208 | 23.955 | 69.364 | 1.00 | 35.39 |
| ATOM | 4021 | CB  | ILE B 222 | 28.961 | 23.069 | 69.244 | 1.00 | 28.31 |
| ATOM | 4022 | CG1 | ILE B 222 | 29.280 | 21.656 | 68.733 | 1.00 | 23.30 |
| ATOM | 4023 | CD1 | ILE B 222 | 28.138 | 20.695 | 68.988 | 1.00 | 31.06 |
| ATOM | 4024 | CG2 | ILE B 222 | 27.871 | 23.684 | 68.394 | 1.00 | 30.00 |
| ATOM | 4025 | C   | ILE B 222 | 29.871 | 25.433 | 69.215 | 1.00 | 31.09 |
| ATOM | 4026 | O   | ILE B 222 | 30.088 | 26.049 | 68.169 | 1.00 | 30.29 |
| ATOM | 4027 | N   | GLN B 223 | 29.352 | 26.009 | 70.296 | 1.00 | 31.17 |
| ATOM | 4028 | CA  | GLN B 223 | 28.973 | 27.416 | 70.289 | 1.00 | 33.58 |
| ATOM | 4029 | CB  | GLN B 223 | 28.201 | 27.804 | 71.554 | 1.00 | 39.47 |
| ATOM | 4030 | CG  | GLN B 223 | 27.198 | 28.916 | 71.237 | 1.00 | 56.44 |
| ATOM | 4031 | CD  | GLN B 223 | 26.886 | 28.937 | 69.747 | 1.00 | 72.62 |
| ATOM | 4032 | OE1 | GLN B 223 | 26.007 | 28.216 | 69.269 | 1.00 | 73.13 |
| ATOM | 4033 | NE2 | GLN B 223 | 27.618 | 29.765 | 69.008 | 1.00 | 86.88 |
| ATOM | 4034 | C   | GLN B 223 | 30.210 | 28.300 | 70.151 | 1.00 | 27.54 |
| ATOM | 4035 | O   | GLN B 223 | 30.195 | 29.217 | 69.338 | 1.00 | 28.05 |
| ATOM | 4036 | N   | PHE B 224 | 31.238 | 27.991 | 70.934 | 1.00 | 26.93 |
| ATOM | 4037 | CA  | PHE B 224 | 32.529 | 28.675 | 70.816 | 1.00 | 21.53 |
| ATOM | 4038 | CB  | PHE B 224 | 33.554 | 28.029 | 71.726 | 1.00 | 22.20 |
| ATOM | 4039 | CG  | PHE B 224 | 34.930 | 28.683 | 71.736 | 1.00 | 25.50 |
| ATOM | 4040 | CD1 | PHE B 224 | 35.141 | 29.892 | 72.381 | 1.00 | 24.49 |
| ATOM | 4041 | CE1 | PHE B 224 | 36.398 | 30.465 | 72.413 | 1.00 | 22.79 |
| ATOM | 4042 | CZ  | PHE B 224 | 37.451 | 29.853 | 71.766 | 1.00 | 14.40 |
| ATOM | 4043 | CE2 | PHE B 224 | 37.260 | 28.650 | 71.125 | 1.00 | 22.52 |
| ATOM | 4044 | CD2 | PHE B 224 | 36.000 | 28.071 | 71.113 | 1.00 | 23.70 |
| ATOM | 4045 | C   | PHE B 224 | 33.033 | 28.659 | 69.372 | 1.00 | 25.07 |
| ATOM | 4046 | O   | PHE B 224 | 33.291 | 29.707 | 68.770 | 1.00 | 33.29 |
| ATOM | 4047 | N   | VAL B 225 | 33.166 | 27.464 | 68.800 | 1.00 | 21.05 |
| ATOM | 4048 | CA  | VAL B 225 | 33.655 | 27.335 | 67.431 | 1.00 | 21.13 |
| ATOM | 4049 | CB  | VAL B 225 | 33.656 | 25.868 | 66.962 | 1.00 | 20.06 |
| ATOM | 4050 | CG1 | VAL B 225 | 33.778 | 25.769 | 65.448 | 1.00 | 21.52 |
| ATOM | 4051 | CG2 | VAL B 225 | 34.796 | 25.101 | 67.607 | 1.00 | 23.47 |
| ATOM | 4052 | C   | VAL B 225 | 32.826 | 28.179 | 66.470 | 1.00 | 34.08 |
| ATOM | 4053 | O   | VAL B 225 | 33.395 | 28.901 | 65.641 | 1.00 | 30.78 |
| ATOM | 4054 | N   | ARG B 226 | 31.498 | 28.088 | 66.584 | 1.00 | 33.79 |
| ATOM | 4055 | CA  | ARG B 226 | 30.663 | 28.875 | 65.670 | 1.00 | 32.97 |

**FIGURE 180**



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4056 | CB  | ARG | B | 226 | 29.185 | 28.551 | 65.852 | 1.00 | 36.13 |
| ATOM | 4057 | CG  | ARG | B | 226 | 28.846 | 27.076 | 65.682 | 1.00 | 38.26 |
| ATOM | 4058 | CD  | ARG | B | 226 | 27.340 | 26.867 | 65.634 | 1.00 | 43.64 |
| ATOM | 4059 | NE  | ARG | B | 226 | 26.967 | 25.743 | 64.773 | 1.00 | 52.04 |
| ATOM | 4060 | CZ  | ARG | B | 226 | 25.960 | 24.913 | 65.031 | 1.00 | 56.46 |
| ATOM | 4061 | NH1 | ARG | B | 226 | 25.229 | 25.084 | 66.127 | 1.00 | 38.23 |
| ATOM | 4062 | NH2 | ARG | B | 226 | 25.688 | 23.917 | 64.197 | 1.00 | 53.92 |
| ATOM | 4063 | C   | ARG | B | 226 | 30.933 | 30.356 | 65.886 | 1.00 | 38.04 |
| ATOM | 4064 | O   | ARG | B | 226 | 31.031 | 31.144 | 64.947 | 1.00 | 40.50 |
| ATOM | 4065 | N   | THR | B | 227 | 31.077 | 30.745 | 67.151 | 1.00 | 32.88 |
| ATOM | 4066 | CA  | THR | B | 227 | 31.406 | 32.146 | 67.425 | 1.00 | 34.79 |
| ATOM | 4067 | CB  | THR | B | 227 | 31.474 | 32.430 | 68.937 | 1.00 | 37.87 |
| ATOM | 4068 | OG1 | THR | B | 227 | 30.160 | 32.368 | 69.504 | 1.00 | 44.90 |
| ATOM | 4069 | CG2 | THR | B | 227 | 31.977 | 33.840 | 69.194 | 1.00 | 37.73 |
| ATOM | 4070 | C   | THR | B | 227 | 32.728 | 32.514 | 66.772 | 1.00 | 33.01 |
| ATOM | 4071 | O   | THR | B | 227 | 32.879 | 33.558 | 66.136 | 1.00 | 29.02 |
| ATOM | 4072 | N   | VAL | B | 228 | 33.737 | 31.645 | 66.903 | 1.00 | 29.04 |
| ATOM | 4073 | CA  | VAL | B | 228 | 35.022 | 32.021 | 66.300 | 1.00 | 25.89 |
| ATOM | 4074 | CB  | VAL | B | 228 | 36.125 | 31.038 | 66.728 | 1.00 | 27.50 |
| ATOM | 4075 | CG1 | VAL | B | 228 | 37.419 | 31.376 | 66.005 | 1.00 | 25.74 |
| ATOM | 4076 | CG2 | VAL | B | 228 | 36.316 | 31.066 | 68.244 | 1.00 | 22.05 |
| ATOM | 4077 | C   | VAL | B | 228 | 34.929 | 32.108 | 64.779 | 1.00 | 25.85 |
| ATOM | 4078 | O   | VAL | B | 228 | 35.454 | 33.028 | 64.145 | 1.00 | 26.36 |
| ATOM | 4079 | N   | ARG | B | 229 | 34.253 | 31.163 | 64.145 | 1.00 | 30.24 |
| ATOM | 4080 | CA  | ARG | B | 229 | 34.172 | 31.158 | 62.678 | 1.00 | 30.97 |
| ATOM | 4081 | CB  | ARG | B | 229 | 33.486 | 29.872 | 62.232 | 1.00 | 35.10 |
| ATOM | 4082 | CG  | ARG | B | 229 | 33.083 | 29.811 | 60.772 | 1.00 | 37.64 |
| ATOM | 4083 | CD  | ARG | B | 229 | 34.250 | 30.014 | 59.828 | 1.00 | 31.83 |
| ATOM | 4084 | NE  | ARG | B | 229 | 35.361 | 29.082 | 60.089 | 1.00 | 32.88 |
| ATOM | 4085 | CZ  | ARG | B | 229 | 36.512 | 29.276 | 59.439 | 1.00 | 32.94 |
| ATOM | 4086 | NH1 | ARG | B | 229 | 36.535 | 30.304 | 58.602 | 1.00 | 27.58 |
| ATOM | 4087 | NH2 | ARG | B | 229 | 37.576 | 28.513 | 59.590 | 1.00 | 33.74 |
| ATOM | 4088 | C   | ARG | B | 229 | 33.459 | 32.398 | 62.160 | 1.00 | 38.61 |
| ATOM | 4089 | O   | ARG | B | 229 | 33.809 | 32.946 | 61.105 | 1.00 | 36.42 |
| ATOM | 4090 | N   | ASP | B | 230 | 32.458 | 32.876 | 62.897 | 1.00 | 30.67 |
| ATOM | 4091 | CA  | ASP | B | 230 | 31.792 | 34.128 | 62.548 | 1.00 | 40.26 |
| ATOM | 4092 | CB  | ASP | B | 230 | 30.693 | 34.455 | 63.561 | 1.00 | 50.06 |
| ATOM | 4093 | CG  | ASP | B | 230 | 29.903 | 35.704 | 63.234 | 1.00 | 61.05 |
| ATOM | 4094 | OD1 | ASP | B | 230 | 30.234 | 36.779 | 63.781 | 1.00 | 62.97 |
| ATOM | 4095 | OD2 | ASP | B | 230 | 28.939 | 35.635 | 62.438 | 1.00 | 74.52 |
| ATOM | 4096 | C   | ASP | B | 230 | 32.777 | 35.287 | 62.469 | 1.00 | 38.62 |
| ATOM | 4097 | O   | ASP | B | 230 | 32.680 | 36.128 | 61.574 | 1.00 | 42.73 |
| ATOM | 4098 | N   | TYR | B | 231 | 33.732 | 35.352 | 63.398 | 1.00 | 33.95 |
| ATOM | 4099 | CA  | TYR | B | 231 | 34.680 | 36.464 | 63.395 | 1.00 | 30.28 |
| ATOM | 4100 | CB  | TYR | B | 231 | 35.391 | 36.596 | 64.743 | 1.00 | 28.40 |
| ATOM | 4101 | CG  | TYR | B | 231 | 34.545 | 37.304 | 65.783 | 1.00 | 31.94 |
| ATOM | 4102 | CD1 | TYR | B | 231 | 33.721 | 36.575 | 66.632 | 1.00 | 31.04 |
| ATOM | 4103 | CE1 | TYR | B | 231 | 32.953 | 37.221 | 67.582 | 1.00 | 39.71 |
| ATOM | 4104 | CZ  | TYR | B | 231 | 33.006 | 38.593 | 67.685 | 1.00 | 44.93 |
| ATOM | 4105 | OH  | TYR | B | 231 | 32.237 | 39.231 | 68.633 | 1.00 | 67.37 |
| ATOM | 4106 | CE2 | TYR | B | 231 | 33.819 | 39.333 | 66.854 | 1.00 | 41.23 |
| ATOM | 4107 | CD2 | TYR | B | 231 | 34.587 | 38.684 | 65.905 | 1.00 | 39.54 |

**FIGURE 181**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4108 | C   | TYR | B | 231 | 35.726 | 36.297 | 62.305 | 1.00 | 28.70 |
| ATOM | 4109 | O   | TYR | B | 231 | 36.213 | 37.238 | 61.692 | 1.00 | 29.85 |
| ATOM | 4110 | N   | ILE | B | 232 | 36.093 | 35.038 | 62.062 | 1.00 | 24.82 |
| ATOM | 4111 | CA  | ILE | B | 232 | 37.053 | 34.819 | 60.989 | 1.00 | 25.65 |
| ATOM | 4112 | CB  | ILE | B | 232 | 37.473 | 33.341 | 60.961 | 1.00 | 22.20 |
| ATOM | 4113 | CG1 | ILE | B | 232 | 38.346 | 32.951 | 62.164 | 1.00 | 25.46 |
| ATOM | 4114 | CD1 | ILE | B | 232 | 38.402 | 31.452 | 62.401 | 1.00 | 22.19 |
| ATOM | 4115 | CG2 | ILE | B | 232 | 38.159 | 32.987 | 59.653 | 1.00 | 26.03 |
| ATOM | 4116 | C   | ILE | B | 232 | 36.450 | 35.262 | 59.657 | 1.00 | 29.68 |
| ATOM | 4117 | O   | ILE | B | 232 | 37.061 | 35.995 | 58.876 | 1.00 | 29.18 |
| ATOM | 4118 | N   | ASN | B | 233 | 35.229 | 34.806 | 59.410 | 1.00 | 29.88 |
| ATOM | 4119 | CA  | ASN | B | 233 | 34.545 | 35.100 | 58.151 | 1.00 | 43.60 |
| ATOM | 4120 | CB  | ASN | B | 233 | 33.148 | 34.472 | 58.179 | 1.00 | 35.22 |
| ATOM | 4121 | CG  | ASN | B | 233 | 33.220 | 32.979 | 57.909 | 1.00 | 32.42 |
| ATOM | 4122 | OD1 | ASN | B | 233 | 34.221 | 32.501 | 57.366 | 1.00 | 44.01 |
| ATOM | 4123 | ND2 | ASN | B | 233 | 32.188 | 32.220 | 58.277 | 1.00 | 29.47 |
| ATOM | 4124 | C   | ASN | B | 233 | 34.512 | 36.604 | 57.892 | 1.00 | 43.88 |
| ATOM | 4125 | O   | ASN | B | 233 | 34.637 | 37.078 | 56.762 | 1.00 | 42.08 |
| ATOM | 4126 | N   | ARG | B | 234 | 34.368 | 37.357 | 58.967 | 1.00 | 40.25 |
| ATOM | 4127 | CA  | ARG | B | 234 | 34.313 | 38.803 | 58.982 | 1.00 | 36.71 |
| ATOM | 4128 | CB  | ARG | B | 234 | 33.385 | 39.259 | 60.130 | 1.00 | 40.64 |
| ATOM | 4129 | CG  | ARG | B | 234 | 31.918 | 39.153 | 59.733 | 1.00 | 50.04 |
| ATOM | 4130 | CD  | ARG | B | 234 | 30.963 | 39.234 | 60.907 | 1.00 | 52.66 |
| ATOM | 4131 | NE  | ARG | B | 234 | 31.267 | 40.346 | 61.795 | 1.00 | 61.93 |
| ATOM | 4132 | CZ  | ARG | B | 234 | 31.331 | 40.270 | 63.116 | 1.00 | 64.33 |
| ATOM | 4133 | NH1 | ARG | B | 234 | 31.107 | 39.119 | 63.732 | 1.00 | 53.92 |
| ATOM | 4134 | NH2 | ARG | B | 234 | 31.619 | 41.352 | 63.825 | 1.00 | 74.42 |
| ATOM | 4135 | C   | ARG | B | 234 | 35.685 | 39.434 | 59.137 | 1.00 | 37.82 |
| ATOM | 4136 | O   | ARG | B | 234 | 35.784 | 40.545 | 59.659 | 1.00 | 49.54 |
| ATOM | 4137 | N   | SER | B | 235 | 36.743 | 38.756 | 58.701 | 1.00 | 31.78 |
| ATOM | 4138 | CA  | SER | B | 235 | 38.087 | 39.304 | 58.815 | 1.00 | 29.31 |
| ATOM | 4139 | CB  | SER | B | 235 | 38.901 | 38.548 | 59.875 | 1.00 | 32.90 |
| ATOM | 4140 | OG  | SER | B | 235 | 38.135 | 38.323 | 61.045 | 1.00 | 44.62 |
| ATOM | 4141 | C   | SER | B | 235 | 38.846 | 39.252 | 57.494 | 1.00 | 35.75 |
| ATOM | 4142 | O   | SER | B | 235 | 39.935 | 38.678 | 57.421 | 1.00 | 35.41 |
| ATOM | 4143 | N   | PRO | B | 236 | 38.319 | 39.848 | 56.436 | 1.00 | 47.17 |
| ATOM | 4144 | CA  | PRO | B | 236 | 38.933 | 39.718 | 55.109 | 1.00 | 44.13 |
| ATOM | 4145 | CB  | PRO | B | 236 | 38.008 | 40.545 | 54.210 | 1.00 | 50.97 |
| ATOM | 4146 | CG  | PRO | B | 236 | 37.355 | 41.506 | 55.150 | 1.00 | 56.25 |
| ATOM | 4147 | CD  | PRO | B | 236 | 37.121 | 40.705 | 56.408 | 1.00 | 56.24 |
| ATOM | 4148 | C   | PRO | B | 236 | 40.345 | 40.289 | 55.070 | 1.00 | 37.49 |
| ATOM | 4149 | O   | PRO | B | 236 | 40.660 | 41.313 | 55.678 | 1.00 | 43.03 |
| ATOM | 4150 | N   | GLY | B | 237 | 41.209 | 39.586 | 54.341 | 1.00 | 33.65 |
| ATOM | 4151 | CA  | GLY | B | 237 | 42.601 | 39.994 | 54.248 | 1.00 | 33.46 |
| ATOM | 4152 | C   | GLY | B | 237 | 43.421 | 39.477 | 55.407 | 1.00 | 26.07 |
| ATOM | 4153 | O   | GLY | B | 237 | 44.630 | 39.670 | 55.500 | 1.00 | 25.20 |
| ATOM | 4154 | N   | ALA | B | 238 | 42.775 | 38.780 | 56.352 | 1.00 | 26.17 |
| ATOM | 4155 | CA  | ALA | B | 238 | 43.611 | 38.252 | 57.430 | 1.00 | 26.70 |
| ATOM | 4156 | CB  | ALA | B | 238 | 42.759 | 37.864 | 58.628 | 1.00 | 26.33 |
| ATOM | 4157 | C   | ALA | B | 238 | 44.430 | 37.058 | 56.946 | 1.00 | 32.60 |
| ATOM | 4158 | O   | ALA | B | 238 | 44.004 | 36.279 | 56.094 | 1.00 | 20.91 |
| ATOM | 4159 | N   | GLY | B | 239 | 45.618 | 36.924 | 57.534 | 1.00 | 28.56 |

**FIGURE 182**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4160 | CA  | GLY | B | 239 | 46.374 | 35.691 | 57.339 | 1.00 | 28.75 |
| ATOM | 4161 | C   | GLY | B | 239 | 45.729 | 34.583 | 58.179 | 1.00 | 23.57 |
| ATOM | 4162 | O   | GLY | B | 239 | 44.556 | 34.686 | 58.553 | 1.00 | 18.99 |
| ATOM | 4163 | N   | PRO | B | 240 | 46.550 | 33.575 | 58.437 | 1.00 | 19.16 |
| ATOM | 4164 | CA  | PRO | B | 240 | 46.088 | 32.396 | 59.170 | 1.00 | 19.17 |
| ATOM | 4165 | CB  | PRO | B | 240 | 47.379 | 31.599 | 59.391 | 1.00 | 21.18 |
| ATOM | 4166 | CG  | PRO | B | 240 | 48.234 | 32.001 | 58.234 | 1.00 | 25.38 |
| ATOM | 4167 | CD  | PRO | B | 240 | 47.974 | 33.480 | 58.072 | 1.00 | 25.67 |
| ATOM | 4168 | C   | PRO | B | 240 | 45.451 | 32.781 | 60.494 | 1.00 | 19.52 |
| ATOM | 4169 | O   | PRO | B | 240 | 45.740 | 33.818 | 61.093 | 1.00 | 24.13 |
| ATOM | 4170 | N   | THR | B | 241 | 44.550 | 31.928 | 60.942 | 1.00 | 18.39 |
| ATOM | 4171 | CA  | THR | B | 241 | 43.980 | 32.007 | 62.281 | 1.00 | 20.07 |
| ATOM | 4172 | CB  | THR | B | 241 | 42.583 | 31.387 | 62.332 | 1.00 | 20.89 |
| ATOM | 4173 | OG1 | THR | B | 241 | 41.622 | 32.194 | 61.631 | 1.00 | 19.78 |
| ATOM | 4174 | CG2 | THR | B | 241 | 42.096 | 31.306 | 63.780 | 1.00 | 20.55 |
| ATOM | 4175 | C   | THR | B | 241 | 44.926 | 31.258 | 63.221 | 1.00 | 23.29 |
| ATOM | 4176 | O   | THR | B | 241 | 45.272 | 30.103 | 62.927 | 1.00 | 13.70 |
| ATOM | 4177 | N   | VAL | B | 242 | 45.381 | 31.875 | 64.316 | 1.00 | 18.05 |
| ATOM | 4178 | CA  | VAL | B | 242 | 46.289 | 31.126 | 65.197 | 1.00 | 19.59 |
| ATOM | 4179 | CB  | VAL | B | 242 | 47.234 | 32.049 | 65.978 | 1.00 | 19.99 |
| ATOM | 4180 | CG1 | VAL | B | 242 | 47.973 | 31.281 | 67.071 | 1.00 | 22.26 |
| ATOM | 4181 | CG2 | VAL | B | 242 | 48.256 | 32.701 | 65.060 | 1.00 | 15.38 |
| ATOM | 4182 | C   | VAL | B | 242 | 45.478 | 30.266 | 66.157 | 1.00 | 17.32 |
| ATOM | 4183 | O   | VAL | B | 242 | 44.453 | 30.702 | 66.663 | 1.00 | 14.54 |
| ATOM | 4184 | N   | VAL | B | 243 | 45.897 | 29.019 | 66.424 | 1.00 | 16.24 |
| ATOM | 4185 | CA  | VAL | B | 243 | 45.166 | 28.247 | 67.444 | 1.00 | 13.16 |
| ATOM | 4186 | CB  | VAL | B | 243 | 44.275 | 27.150 | 66.860 | 1.00 | 15.05 |
| ATOM | 4187 | CG1 | VAL | B | 243 | 43.399 | 26.461 | 67.922 | 1.00 | 13.07 |
| ATOM | 4188 | CG2 | VAL | B | 243 | 43.389 | 27.729 | 65.760 | 1.00 | 10.83 |
| ATOM | 4189 | C   | VAL | B | 243 | 46.218 | 27.641 | 68.355 | 1.00 | 12.85 |
| ATOM | 4190 | O   | VAL | B | 243 | 47.232 | 27.116 | 67.875 | 1.00 | 13.00 |
| ATOM | 4191 | N   | HIS | B | 244 | 46.034 | 27.683 | 69.667 | 1.00 | 17.27 |
| ATOM | 4192 | CA  | HIS | B | 244 | 47.023 | 27.037 | 70.522 | 1.00 | 14.69 |
| ATOM | 4193 | CB  | HIS | B | 244 | 48.209 | 27.931 | 70.868 | 1.00 | 17.49 |
| ATOM | 4194 | CG  | HIS | B | 244 | 47.942 | 28.983 | 71.909 | 1.00 | 22.46 |
| ATOM | 4195 | ND1 | HIS | B | 244 | 48.065 | 28.773 | 73.260 | 1.00 | 18.81 |
| ATOM | 4196 | CE1 | HIS | B | 244 | 47.778 | 29.877 | 73.925 | 1.00 | 16.49 |
| ATOM | 4197 | NE2 | HIS | B | 244 | 47.471 | 30.820 | 73.044 | 1.00 | 20.57 |
| ATOM | 4198 | CD2 | HIS | B | 244 | 47.576 | 30.286 | 71.781 | 1.00 | 22.25 |
| ATOM | 4199 | C   | HIS | B | 244 | 46.349 | 26.574 | 71.821 | 1.00 | 12.09 |
| ATOM | 4200 | O   | HIS | B | 244 | 45.286 | 27.061 | 72.168 | 1.00 | 14.03 |
| ATOM | 4201 | N   | CYS | B | 245 | 47.029 | 25.631 | 72.434 | 1.00 | 16.27 |
| ATOM | 4202 | CA  | CYS | B | 245 | 46.655 | 25.083 | 73.747 | 1.00 | 15.96 |
| ATOM | 4203 | CB  | CYS | B | 245 | 45.929 | 23.756 | 73.577 | 1.00 | 24.17 |
| ATOM | 4204 | SG  | CYS | B | 245 | 46.767 | 22.530 | 72.540 | 1.00 | 19.97 |
| ATOM | 4205 | C   | CYS | B | 245 | 47.952 | 25.010 | 74.536 | 1.00 | 23.79 |
| ATOM | 4206 | O   | CYS | B | 245 | 48.651 | 26.039 | 74.621 | 1.00 | 17.71 |
| ATOM | 4207 | N   | SER | B | 246 | 48.357 | 23.869 | 75.088 | 1.00 | 15.26 |
| ATOM | 4208 | CA  | SER | B | 246 | 49.645 | 23.864 | 75.785 | 1.00 | 15.41 |
| ATOM | 4209 | CB  | SER | B | 246 | 49.587 | 23.047 | 77.091 | 1.00 | 8.58  |
| ATOM | 4210 | OG  | SER | B | 246 | 50.839 | 23.185 | 77.745 | 1.00 | 14.15 |
| ATOM | 4211 | C   | SER | B | 246 | 50.725 | 23.332 | 74.858 | 1.00 | 19.97 |

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FIGURE 183

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 4212 | O   | SER B 246 | 51.746 | 23.963 | 74.592 | 1.00 | 14.07 |
| ATOM | 4213 | N   | ALA B 247 | 50.505 | 22.130 | 74.328 | 1.00 | 17.84 |
| ATOM | 4214 | CA  | ALA B 247 | 51.486 | 21.562 | 73.428 | 1.00 | 12.20 |
| ATOM | 4215 | CB  | ALA B 247 | 51.563 | 20.047 | 73.532 | 1.00 | 18.43 |
| ATOM | 4216 | C   | ALA B 247 | 51.157 | 21.898 | 71.970 | 1.00 | 13.39 |
| ATOM | 4217 | O   | ALA B 247 | 52.039 | 21.689 | 71.133 | 1.00 | 21.82 |
| ATOM | 4218 | N   | GLY B 248 | 49.949 | 22.376 | 71.712 | 1.00 | 11.10 |
| ATOM | 4219 | CA  | GLY B 248 | 49.513 | 22.677 | 70.361 | 1.00 | 14.48 |
| ATOM | 4220 | C   | GLY B 248 | 49.114 | 21.449 | 69.571 | 1.00 | 26.17 |
| ATOM | 4221 | O   | GLY B 248 | 49.288 | 21.419 | 68.350 | 1.00 | 26.33 |
| ATOM | 4222 | N   | VAL B 249 | 48.574 | 20.398 | 70.200 | 1.00 | 19.25 |
| ATOM | 4223 | CA  | VAL B 249 | 48.239 | 19.232 | 69.365 | 1.00 | 19.23 |
| ATOM | 4224 | CB  | VAL B 249 | 49.293 | 18.114 | 69.401 | 1.00 | 18.92 |
| ATOM | 4225 | CG1 | VAL B 249 | 50.682 | 18.568 | 68.977 | 1.00 | 15.44 |
| ATOM | 4226 | CG2 | VAL B 249 | 49.432 | 17.478 | 70.794 | 1.00 | 20.80 |
| ATOM | 4227 | C   | VAL B 249 | 46.884 | 18.672 | 69.748 | 1.00 | 16.22 |
| ATOM | 4228 | O   | VAL B 249 | 46.010 | 18.434 | 68.890 | 1.00 | 22.29 |
| ATOM | 4229 | N   | GLY B 250 | 46.602 | 18.422 | 71.030 | 1.00 | 21.24 |
| ATOM | 4230 | CA  | GLY B 250 | 45.334 | 17.751 | 71.313 | 1.00 | 23.25 |
| ATOM | 4231 | C   | GLY B 250 | 44.109 | 18.612 | 71.266 | 1.00 | 24.10 |
| ATOM | 4232 | O   | GLY B 250 | 43.159 | 18.477 | 70.484 | 1.00 | 21.30 |
| ATOM | 4233 | N   | ARG B 251 | 44.071 | 19.606 | 72.170 | 1.00 | 12.60 |
| ATOM | 4234 | CA  | ARG B 251 | 42.891 | 20.459 | 72.174 | 1.00 | 14.08 |
| ATOM | 4235 | CB  | ARG B 251 | 42.941 | 21.317 | 73.449 | 1.00 | 17.84 |
| ATOM | 4236 | CG  | ARG B 251 | 42.681 | 20.419 | 74.664 | 1.00 | 18.30 |
| ATOM | 4237 | CD  | ARG B 251 | 42.862 | 21.184 | 75.963 | 1.00 | 15.33 |
| ATOM | 4238 | NE  | ARG B 251 | 44.280 | 21.335 | 76.262 | 1.00 | 21.24 |
| ATOM | 4239 | CZ  | ARG B 251 | 44.713 | 22.030 | 77.317 | 1.00 | 22.30 |
| ATOM | 4240 | NH1 | ARG B 251 | 43.820 | 22.588 | 78.124 | 1.00 | 18.21 |
| ATOM | 4241 | NH2 | ARG B 251 | 46.013 | 22.129 | 77.516 | 1.00 | 17.67 |
| ATOM | 4242 | C   | ARG B 251 | 42.869 | 21.322 | 70.928 | 1.00 | 18.05 |
| ATOM | 4243 | O   | ARG B 251 | 41.815 | 21.598 | 70.358 | 1.00 | 21.59 |
| ATOM | 4244 | N   | THR B 252 | 44.086 | 21.740 | 70.545 | 1.00 | 14.56 |
| ATOM | 4245 | CA  | THR B 252 | 44.135 | 22.560 | 69.328 | 1.00 | 21.90 |
| ATOM | 4246 | CB  | THR B 252 | 45.580 | 23.025 | 69.081 | 1.00 | 21.05 |
| ATOM | 4247 | OG1 | THR B 252 | 45.872 | 24.089 | 70.001 | 1.00 | 21.60 |
| ATOM | 4248 | CG2 | THR B 252 | 45.705 | 23.561 | 67.670 | 1.00 | 19.25 |
| ATOM | 4249 | C   | THR B 252 | 43.600 | 21.794 | 68.120 | 1.00 | 21.20 |
| ATOM | 4250 | O   | THR B 252 | 42.811 | 22.292 | 67.312 | 1.00 | 19.48 |
| ATOM | 4251 | N   | GLY B 253 | 44.043 | 20.545 | 68.002 | 1.00 | 22.67 |
| ATOM | 4252 | CA  | GLY B 253 | 43.671 | 19.713 | 66.862 | 1.00 | 16.29 |
| ATOM | 4253 | C   | GLY B 253 | 42.198 | 19.395 | 66.821 | 1.00 | 22.35 |
| ATOM | 4254 | O   | GLY B 253 | 41.587 | 19.330 | 65.747 | 1.00 | 19.39 |
| ATOM | 4255 | N   | THR B 254 | 41.634 | 19.191 | 68.022 | 1.00 | 25.18 |
| ATOM | 4256 | CA  | THR B 254 | 40.194 | 18.939 | 68.106 | 1.00 | 15.84 |
| ATOM | 4257 | CB  | THR B 254 | 39.805 | 18.402 | 69.499 | 1.00 | 21.21 |
| ATOM | 4258 | OG1 | THR B 254 | 40.624 | 17.266 | 69.796 | 1.00 | 19.04 |
| ATOM | 4259 | CG2 | THR B 254 | 38.361 | 17.943 | 69.525 | 1.00 | 24.29 |
| ATOM | 4260 | C   | THR B 254 | 39.422 | 20.198 | 67.781 | 1.00 | 19.07 |
| ATOM | 4261 | O   | THR B 254 | 38.352 | 20.162 | 67.182 | 1.00 | 21.18 |
| ATOM | 4262 | N   | PHE B 255 | 39.931 | 21.367 | 68.178 | 1.00 | 21.95 |
| ATOM | 4263 | CA  | PHE B 255 | 39.225 | 22.595 | 67.821 | 1.00 | 22.07 |

**FIGURE 184**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4264 | CB  | PHE | B | 255 | 39.910 | 23.855 | 68.368 | 1.00 | 20.64 |
| ATOM | 4265 | CG  | PHE | B | 255 | 39.280 | 25.177 | 67.939 | 1.00 | 16.94 |
| ATOM | 4266 | CD1 | PHE | B | 255 | 38.222 | 25.716 | 68.650 | 1.00 | 17.36 |
| ATOM | 4267 | CE1 | PHE | B | 255 | 37.628 | 26.901 | 68.272 | 1.00 | 16.83 |
| ATOM | 4268 | CZ  | PHE | B | 255 | 38.079 | 27.576 | 67.156 | 1.00 | 20.63 |
| ATOM | 4269 | CE2 | PHE | B | 255 | 39.141 | 27.067 | 66.427 | 1.00 | 15.59 |
| ATOM | 4270 | CD2 | PHE | B | 255 | 39.730 | 25.892 | 66.841 | 1.00 | 26.52 |
| ATOM | 4271 | C   | PHE | B | 255 | 39.148 | 22.712 | 66.298 | 1.00 | 16.89 |
| ATOM | 4272 | O   | PHE | B | 255 | 38.114 | 23.045 | 65.727 | 1.00 | 22.55 |
| ATOM | 4273 | N   | ILE | B | 256 | 40.305 | 22.497 | 65.682 | 1.00 | 22.37 |
| ATOM | 4274 | CA  | ILE | B | 256 | 40.393 | 22.694 | 64.232 | 1.00 | 26.45 |
| ATOM | 4275 | CB  | ILE | B | 256 | 41.841 | 22.644 | 63.742 | 1.00 | 22.17 |
| ATOM | 4276 | CG1 | ILE | B | 256 | 42.717 | 23.802 | 64.245 | 1.00 | 19.09 |
| ATOM | 4277 | CD1 | ILE | B | 256 | 44.182 | 23.636 | 63.845 | 1.00 | 17.45 |
| ATOM | 4278 | CG2 | ILE | B | 256 | 41.861 | 22.570 | 62.218 | 1.00 | 25.40 |
| ATOM | 4279 | C   | ILE | B | 256 | 39.556 | 21.645 | 63.513 | 1.00 | 25.61 |
| ATOM | 4280 | O   | ILE | B | 256 | 38.871 | 21.935 | 62.537 | 1.00 | 32.43 |
| ATOM | 4281 | N   | ALA | B | 257 | 39.588 | 20.418 | 64.006 | 1.00 | 22.52 |
| ATOM | 4282 | CA  | ALA | B | 257 | 38.740 | 19.395 | 63.390 | 1.00 | 28.35 |
| ATOM | 4283 | CB  | ALA | B | 257 | 39.011 | 18.049 | 64.057 | 1.00 | 23.53 |
| ATOM | 4284 | C   | ALA | B | 257 | 37.271 | 19.768 | 63.462 | 1.00 | 31.55 |
| ATOM | 4285 | O   | ALA | B | 257 | 36.495 | 19.520 | 62.536 | 1.00 | 36.42 |
| ATOM | 4286 | N   | LEU | B | 258 | 36.833 | 20.366 | 64.568 | 1.00 | 27.78 |
| ATOM | 4287 | CA  | LEU | B | 258 | 35.425 | 20.714 | 64.735 | 1.00 | 25.99 |
| ATOM | 4288 | CB  | LEU | B | 258 | 35.101 | 21.046 | 66.201 | 1.00 | 29.85 |
| ATOM | 4289 | CG  | LEU | B | 258 | 33.612 | 21.160 | 66.530 | 1.00 | 31.93 |
| ATOM | 4290 | CD1 | LEU | B | 258 | 32.852 | 19.931 | 66.050 | 1.00 | 21.42 |
| ATOM | 4291 | CD2 | LEU | B | 258 | 33.381 | 21.372 | 68.020 | 1.00 | 29.92 |
| ATOM | 4292 | C   | LEU | B | 258 | 35.049 | 21.898 | 63.862 | 1.00 | 28.98 |
| ATOM | 4293 | O   | LEU | B | 258 | 33.955 | 21.967 | 63.306 | 1.00 | 33.28 |
| ATOM | 4294 | N   | ASP | B | 259 | 35.976 | 22.850 | 63.743 | 1.00 | 25.38 |
| ATOM | 4295 | CA  | ASP | B | 259 | 35.725 | 23.991 | 62.856 | 1.00 | 26.70 |
| ATOM | 4296 | CB  | ASP | B | 259 | 36.911 | 24.943 | 62.895 | 1.00 | 25.83 |
| ATOM | 4297 | CG  | ASP | B | 259 | 36.704 | 26.266 | 62.193 | 1.00 | 34.39 |
| ATOM | 4298 | OD1 | ASP | B | 259 | 35.615 | 26.855 | 62.335 | 1.00 | 28.39 |
| ATOM | 4299 | OD2 | ASP | B | 259 | 37.650 | 26.717 | 61.505 | 1.00 | 32.58 |
| ATOM | 4300 | C   | ASP | B | 259 | 35.466 | 23.504 | 61.433 | 1.00 | 19.95 |
| ATOM | 4301 | O   | ASP | B | 259 | 34.559 | 23.983 | 60.753 | 1.00 | 32.03 |
| ATOM | 4302 | N   | ARG | B | 260 | 36.261 | 22.532 | 60.984 | 1.00 | 24.53 |
| ATOM | 4303 | CA  | ARG | B | 260 | 36.087 | 22.057 | 59.603 | 1.00 | 25.87 |
| ATOM | 4304 | CB  | ARG | B | 260 | 37.297 | 21.239 | 59.169 | 1.00 | 26.24 |
| ATOM | 4305 | CG  | ARG | B | 260 | 38.591 | 22.045 | 59.058 | 1.00 | 28.14 |
| ATOM | 4306 | CD  | ARG | B | 260 | 39.709 | 21.131 | 58.569 | 1.00 | 24.62 |
| ATOM | 4307 | NE  | ARG | B | 260 | 39.311 | 20.472 | 57.320 | 1.00 | 31.53 |
| ATOM | 4308 | CZ  | ARG | B | 260 | 40.177 | 20.214 | 56.345 | 1.00 | 39.36 |
| ATOM | 4309 | NH1 | ARG | B | 260 | 41.447 | 20.563 | 56.493 | 1.00 | 41.26 |
| ATOM | 4310 | NH2 | ARG | B | 260 | 39.778 | 19.617 | 55.231 | 1.00 | 56.76 |
| ATOM | 4311 | C   | ARG | B | 260 | 34.822 | 21.239 | 59.447 | 1.00 | 31.74 |
| ATOM | 4312 | O   | ARG | B | 260 | 34.189 | 21.251 | 58.392 | 1.00 | 39.13 |
| ATOM | 4313 | N   | ILE | B | 261 | 34.381 | 20.492 | 60.468 | 1.00 | 30.98 |
| ATOM | 4314 | CA  | ILE | B | 261 | 33.208 | 19.657 | 60.165 | 1.00 | 35.76 |
| ATOM | 4315 | CB  | ILE | B | 261 | 33.146 | 18.381 | 61.023 | 1.00 | 33.31 |

**FIGURE 185**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 4316 | CG1 | ILE | B | 261 | 32.912 | 18.576 | 62.521 | 1.00 | 27.49  |
| ATOM | 4317 | CD1 | ILE | B | 261 | 33.493 | 17.459 | 63.368 | 1.00 | 32.91  |
| ATOM | 4318 | CG2 | ILE | B | 261 | 34.414 | 17.561 | 60.796 | 1.00 | 33.85  |
| ATOM | 4319 | C   | ILE | B | 261 | 31.938 | 20.476 | 60.307 | 1.00 | 41.61  |
| ATOM | 4320 | O   | ILE | B | 261 | 30.932 | 20.212 | 59.641 | 1.00 | 42.61  |
| ATOM | 4321 | N   | LEU | B | 262 | 31.977 | 21.494 | 61.170 | 1.00 | 36.25  |
| ATOM | 4322 | CA  | LEU | B | 262 | 30.747 | 22.281 | 61.321 | 1.00 | 37.79  |
| ATOM | 4323 | CB  | LEU | B | 262 | 30.868 | 23.297 | 62.448 | 1.00 | 33.16  |
| ATOM | 4324 | CG  | LEU | B | 262 | 30.867 | 22.707 | 63.865 | 1.00 | 34.98  |
| ATOM | 4325 | CD1 | LEU | B | 262 | 30.730 | 23.791 | 64.918 | 1.00 | 35.24  |
| ATOM | 4326 | CD2 | LEU | B | 262 | 29.751 | 21.680 | 64.011 | 1.00 | 39.50  |
| ATOM | 4327 | C   | LEU | B | 262 | 30.444 | 22.945 | 59.982 | 1.00 | 48.10  |
| ATOM | 4328 | O   | LEU | B | 262 | 29.297 | 23.137 | 59.592 | 1.00 | 54.41  |
| ATOM | 4329 | N   | GLN | B | 263 | 31.536 | 23.268 | 59.294 | 1.00 | 42.55  |
| ATOM | 4330 | CA  | GLN | B | 263 | 31.446 | 23.852 | 57.963 | 1.00 | 45.39  |
| ATOM | 4331 | CB  | GLN | B | 263 | 32.819 | 24.403 | 57.562 | 1.00 | 47.06  |
| ATOM | 4332 | CG  | GLN | B | 263 | 33.160 | 25.695 | 58.293 | 1.00 | 52.92  |
| ATOM | 4333 | CD  | GLN | B | 263 | 34.546 | 26.217 | 57.972 | 1.00 | 51.62  |
| ATOM | 4334 | OE1 | GLN | B | 263 | 34.689 | 27.171 | 57.208 | 1.00 | 48.47  |
| ATOM | 4335 | NE2 | GLN | B | 263 | 35.575 | 25.609 | 58.552 | 1.00 | 34.73  |
| ATOM | 4336 | C   | GLN | B | 263 | 30.935 | 22.825 | 56.961 | 1.00 | 37.20  |
| ATOM | 4337 | O   | GLN | B | 263 | 29.987 | 23.076 | 56.223 | 1.00 | 36.52  |
| ATOM | 4338 | N   | GLN | B | 264 | 31.551 | 21.651 | 56.930 | 1.00 | 48.77  |
| ATOM | 4339 | CA  | GLN | B | 264 | 31.089 | 20.583 | 56.052 | 1.00 | 54.55  |
| ATOM | 4340 | CB  | GLN | B | 264 | 31.890 | 19.305 | 56.289 | 1.00 | 51.39  |
| ATOM | 4341 | CG  | GLN | B | 264 | 33.377 | 19.395 | 55.996 | 1.00 | 45.82  |
| ATOM | 4342 | CD  | GLN | B | 264 | 34.080 | 18.072 | 56.248 | 1.00 | 49.30  |
| ATOM | 4343 | OE1 | GLN | B | 264 | 33.426 | 17.046 | 56.440 | 1.00 | 54.85  |
| ATOM | 4344 | NE2 | GLN | B | 264 | 35.410 | 18.093 | 56.256 | 1.00 | 42.52  |
| ATOM | 4345 | C   | GLN | B | 264 | 29.602 | 20.309 | 56.268 | 1.00 | 65.82  |
| ATOM | 4346 | O   | GLN | B | 264 | 28.854 | 20.101 | 55.312 | 1.00 | 71.36  |
| ATOM | 4347 | N   | LEU | B | 265 | 29.169 | 20.311 | 57.529 | 1.00 | 66.58  |
| ATOM | 4348 | CA  | LEU | B | 265 | 27.766 | 20.033 | 57.816 | 1.00 | 67.06  |
| ATOM | 4349 | CB  | LEU | B | 265 | 27.465 | 20.150 | 59.309 | 1.00 | 67.27  |
| ATOM | 4350 | CG  | LEU | B | 265 | 27.604 | 18.870 | 60.130 | 1.00 | 71.80  |
| ATOM | 4351 | CD1 | LEU | B | 265 | 27.000 | 19.066 | 61.515 | 1.00 | 69.10  |
| ATOM | 4352 | CD2 | LEU | B | 265 | 26.955 | 17.695 | 59.409 | 1.00 | 78.85  |
| ATOM | 4353 | C   | LEU | B | 265 | 26.858 | 20.996 | 57.055 | 1.00 | 65.79  |
| ATOM | 4354 | O   | LEU | B | 265 | 25.951 | 20.581 | 56.340 | 1.00 | 62.34  |
| ATOM | 4355 | N   | ASP | B | 266 | 27.140 | 22.278 | 57.242 | 1.00 | 61.77  |
| ATOM | 4356 | CA  | ASP | B | 266 | 26.333 | 23.341 | 56.663 | 1.00 | 64.82  |
| ATOM | 4357 | CB  | ASP | B | 266 | 26.740 | 24.673 | 57.312 | 1.00 | 71.48  |
| ATOM | 4358 | CG  | ASP | B | 266 | 26.589 | 24.603 | 58.822 | 1.00 | 82.79  |
| ATOM | 4359 | OD1 | ASP | B | 266 | 26.033 | 23.597 | 59.312 | 1.00 | 89.00  |
| ATOM | 4360 | OD2 | ASP | B | 266 | 27.021 | 25.562 | 59.500 | 1.00 | 104.58 |
| ATOM | 4361 | C   | ASP | B | 266 | 26.454 | 23.433 | 55.152 | 1.00 | 62.69  |
| ATOM | 4362 | O   | ASP | B | 266 | 25.779 | 24.251 | 54.519 | 1.00 | 61.16  |
| ATOM | 4363 | N   | SER | B | 267 | 27.294 | 22.612 | 54.520 | 1.00 | 56.01  |
| ATOM | 4364 | CA  | SER | B | 267 | 27.375 | 22.733 | 53.063 | 1.00 | 54.60  |
| ATOM | 4365 | CB  | SER | B | 267 | 28.557 | 23.647 | 52.720 | 1.00 | 53.27  |
| ATOM | 4366 | OG  | SER | B | 267 | 29.698 | 23.231 | 53.454 | 1.00 | 48.03  |
| ATOM | 4367 | C   | SER | B | 267 | 27.529 | 21.401 | 52.353 | 1.00 | 61.19  |

**FIGURE 186**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 4368 | O   | SER | B | 267 | 27.489 | 21.325 | 51.121 | 1.00 | 78.99  |
| ATOM | 4369 | N   | LYS | B | 268 | 27.711 | 20.321 | 53.101 | 1.00 | 66.12  |
| ATOM | 4370 | CA  | LYS | B | 268 | 27.946 | 19.017 | 52.481 | 1.00 | 67.60  |
| ATOM | 4371 | CB  | LYS | B | 268 | 29.387 | 18.583 | 52.742 | 1.00 | 73.63  |
| ATOM | 4372 | CG  | LYS | B | 268 | 29.798 | 17.277 | 52.087 | 1.00 | 76.35  |
| ATOM | 4373 | CD  | LYS | B | 268 | 31.310 | 17.139 | 52.000 | 1.00 | 69.59  |
| ATOM | 4374 | CE  | LYS | B | 268 | 31.983 | 17.228 | 53.356 | 1.00 | 57.88  |
| ATOM | 4375 | NZ  | LYS | B | 268 | 32.516 | 15.916 | 53.815 | 1.00 | 46.13  |
| ATOM | 4376 | C   | LYS | B | 268 | 26.957 | 17.982 | 52.997 | 1.00 | 59.94  |
| ATOM | 4377 | O   | LYS | B | 268 | 26.428 | 18.102 | 54.100 | 1.00 | 64.53  |
| ATOM | 4378 | N   | ASP | B | 269 | 26.692 | 16.955 | 52.201 | 1.00 | 56.14  |
| ATOM | 4379 | CA  | ASP | B | 269 | 25.749 | 15.913 | 52.591 | 1.00 | 60.87  |
| ATOM | 4380 | CB  | ASP | B | 269 | 24.980 | 15.392 | 51.377 | 1.00 | 71.26  |
| ATOM | 4381 | CG  | ASP | B | 269 | 25.670 | 15.678 | 50.060 | 1.00 | 82.48  |
| ATOM | 4382 | OD1 | ASP | B | 269 | 26.027 | 16.846 | 49.797 | 1.00 | 101.89 |
| ATOM | 4383 | OD2 | ASP | B | 269 | 25.856 | 14.725 | 49.273 | 1.00 | 103.90 |
| ATOM | 4384 | C   | ASP | B | 269 | 26.479 | 14.771 | 53.294 | 1.00 | 57.30  |
| ATOM | 4385 | O   | ASP | B | 269 | 25.869 | 13.797 | 53.732 | 1.00 | 54.94  |
| ATOM | 4386 | N   | SER | B | 270 | 27.797 | 14.922 | 53.393 | 1.00 | 44.67  |
| ATOM | 4387 | CA  | SER | B | 270 | 28.633 | 13.990 | 54.132 | 1.00 | 41.73  |
| ATOM | 4388 | CB  | SER | B | 270 | 29.526 | 13.168 | 53.206 | 1.00 | 43.00  |
| ATOM | 4389 | OG  | SER | B | 270 | 28.790 | 12.556 | 52.162 | 1.00 | 51.47  |
| ATOM | 4390 | C   | SER | B | 270 | 29.487 | 14.760 | 55.142 | 1.00 | 42.93  |
| ATOM | 4391 | O   | SER | B | 270 | 29.563 | 15.988 | 55.100 | 1.00 | 44.44  |
| ATOM | 4392 | N   | VAL | B | 271 | 30.122 | 14.024 | 56.045 | 1.00 | 39.47  |
| ATOM | 4393 | CA  | VAL | B | 271 | 31.033 | 14.606 | 57.020 | 1.00 | 42.42  |
| ATOM | 4394 | CB  | VAL | B | 271 | 30.399 | 14.754 | 58.412 | 1.00 | 43.26  |
| ATOM | 4395 | CG1 | VAL | B | 271 | 29.733 | 13.460 | 58.864 | 1.00 | 32.79  |
| ATOM | 4396 | CG2 | VAL | B | 271 | 31.460 | 15.183 | 59.417 | 1.00 | 35.29  |
| ATOM | 4397 | C   | VAL | B | 271 | 32.282 | 13.735 | 57.095 | 1.00 | 48.99  |
| ATOM | 4398 | O   | VAL | B | 271 | 32.184 | 12.509 | 57.041 | 1.00 | 58.21  |
| ATOM | 4399 | N   | ASP | B | 272 | 33.444 | 14.367 | 57.209 | 1.00 | 45.99  |
| ATOM | 4400 | CA  | ASP | B | 272 | 34.707 | 13.648 | 57.135 | 1.00 | 35.10  |
| ATOM | 4401 | CB  | ASP | B | 272 | 35.417 | 14.055 | 55.832 | 1.00 | 36.44  |
| ATOM | 4402 | CG  | ASP | B | 272 | 36.191 | 12.901 | 55.232 | 1.00 | 35.96  |
| ATOM | 4403 | OD1 | ASP | B | 272 | 36.367 | 11.892 | 55.943 | 1.00 | 46.07  |
| ATOM | 4404 | OD2 | ASP | B | 272 | 36.621 | 13.010 | 54.067 | 1.00 | 60.29  |
| ATOM | 4405 | C   | ASP | B | 272 | 35.605 | 13.897 | 58.334 | 1.00 | 38.48  |
| ATOM | 4406 | O   | ASP | B | 272 | 36.631 | 14.567 | 58.238 | 1.00 | 37.38  |
| ATOM | 4407 | N   | ILE | B | 273 | 35.225 | 13.349 | 59.485 | 1.00 | 44.55  |
| ATOM | 4408 | CA  | ILE | B | 273 | 36.018 | 13.484 | 60.706 | 1.00 | 42.80  |
| ATOM | 4409 | CB  | ILE | B | 273 | 35.239 | 12.986 | 61.941 | 1.00 | 44.89  |
| ATOM | 4410 | CG1 | ILE | B | 273 | 34.010 | 13.836 | 62.283 | 1.00 | 43.95  |
| ATOM | 4411 | CD1 | ILE | B | 273 | 32.873 | 13.080 | 62.950 | 1.00 | 28.68  |
| ATOM | 4412 | CG2 | ILE | B | 273 | 36.135 | 12.859 | 63.164 | 1.00 | 35.00  |
| ATOM | 4413 | C   | ILE | B | 273 | 37.341 | 12.749 | 60.554 | 1.00 | 43.03  |
| ATOM | 4414 | O   | ILE | B | 273 | 38.397 | 13.283 | 60.903 | 1.00 | 47.22  |
| ATOM | 4415 | N   | TYR | B | 274 | 37.333 | 11.528 | 60.019 | 1.00 | 33.68  |
| ATOM | 4416 | CA  | TYR | B | 274 | 38.587 | 10.824 | 59.758 | 1.00 | 33.83  |
| ATOM | 4417 | CB  | TYR | B | 274 | 38.323 | 9.463  | 59.101 | 1.00 | 31.32  |
| ATOM | 4418 | CG  | TYR | B | 274 | 39.536 | 8.615  | 58.815 | 1.00 | 34.21  |
| ATOM | 4419 | CD1 | TYR | B | 274 | 40.011 | 7.706  | 59.752 | 1.00 | 27.81  |

**FIGURE 187**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4420 | CE1 | TYR | B | 274 | 41.124 | 6.936  | 59.481 | 1.00 | 33.31 |
| ATOM | 4421 | CZ  | TYR | B | 274 | 41.783 | 7.051  | 58.280 | 1.00 | 38.03 |
| ATOM | 4422 | OH  | TYR | B | 274 | 42.894 | 6.287  | 57.994 | 1.00 | 74.99 |
| ATOM | 4423 | CE2 | TYR | B | 274 | 41.334 | 7.942  | 57.338 | 1.00 | 34.20 |
| ATOM | 4424 | CD2 | TYR | B | 274 | 40.227 | 8.704  | 57.615 | 1.00 | 30.48 |
| ATOM | 4425 | C   | TYR | B | 274 | 39.499 | 11.654 | 58.857 | 1.00 | 30.77 |
| ATOM | 4426 | O   | TYR | B | 274 | 40.699 | 11.762 | 59.091 | 1.00 | 42.32 |
| ATOM | 4427 | N   | GLY | B | 275 | 38.914 | 12.201 | 57.796 | 1.00 | 33.93 |
| ATOM | 4428 | CA  | GLY | B | 275 | 39.661 | 12.924 | 56.786 | 1.00 | 34.96 |
| ATOM | 4429 | C   | GLY | B | 275 | 40.242 | 14.213 | 57.340 | 1.00 | 28.44 |
| ATOM | 4430 | O   | GLY | B | 275 | 41.328 | 14.628 | 56.928 | 1.00 | 26.09 |
| ATOM | 4431 | N   | ALA | B | 276 | 39.508 | 14.838 | 58.264 | 1.00 | 30.51 |
| ATOM | 4432 | CA  | ALA | B | 276 | 40.037 | 16.083 | 58.849 | 1.00 | 32.53 |
| ATOM | 4433 | CB  | ALA | B | 276 | 38.977 | 16.819 | 59.633 | 1.00 | 28.84 |
| ATOM | 4434 | C   | ALA | B | 276 | 41.233 | 15.754 | 59.724 | 1.00 | 28.27 |
| ATOM | 4435 | O   | ALA | B | 276 | 42.298 | 16.355 | 59.634 | 1.00 | 27.29 |
| ATOM | 4436 | N   | VAL | B | 277 | 41.052 | 14.745 | 60.587 | 1.00 | 22.62 |
| ATOM | 4437 | CA  | VAL | B | 277 | 42.157 | 14.409 | 61.478 | 1.00 | 22.13 |
| ATOM | 4438 | CB  | VAL | B | 277 | 41.713 | 13.420 | 62.569 | 1.00 | 25.76 |
| ATOM | 4439 | CG1 | VAL | B | 277 | 42.931 | 12.861 | 63.293 | 1.00 | 33.74 |
| ATOM | 4440 | CG2 | VAL | B | 277 | 40.769 | 14.087 | 63.561 | 1.00 | 22.07 |
| ATOM | 4441 | C   | VAL | B | 277 | 43.342 | 13.846 | 60.712 | 1.00 | 31.87 |
| ATOM | 4442 | O   | VAL | B | 277 | 44.512 | 14.018 | 61.076 | 1.00 | 30.97 |
| ATOM | 4443 | N   | HIS | B | 278 | 43.053 | 13.141 | 59.616 | 1.00 | 26.49 |
| ATOM | 4444 | CA  | HIS | B | 278 | 44.180 | 12.632 | 58.831 | 1.00 | 24.97 |
| ATOM | 4445 | CB  | HIS | B | 278 | 43.663 | 11.735 | 57.699 | 1.00 | 26.29 |
| ATOM | 4446 | CG  | HIS | B | 278 | 44.716 | 11.393 | 56.689 | 1.00 | 35.64 |
| ATOM | 4447 | ND1 | HIS | B | 278 | 45.145 | 12.273 | 55.723 | 1.00 | 32.18 |
| ATOM | 4448 | CE1 | HIS | B | 278 | 46.077 | 11.699 | 54.986 | 1.00 | 36.91 |
| ATOM | 4449 | NE2 | HIS | B | 278 | 46.280 | 10.473 | 55.443 | 1.00 | 39.75 |
| ATOM | 4450 | CD2 | HIS | B | 278 | 45.440 | 10.261 | 56.509 | 1.00 | 40.27 |
| ATOM | 4451 | C   | HIS | B | 278 | 44.988 | 13.809 | 58.294 | 1.00 | 17.49 |
| ATOM | 4452 | O   | HIS | B | 278 | 46.212 | 13.862 | 58.377 | 1.00 | 21.10 |
| ATOM | 4453 | N   | ASP | B | 279 | 44.262 | 14.777 | 57.736 | 1.00 | 23.86 |
| ATOM | 4454 | CA  | ASP | B | 279 | 44.908 | 15.964 | 57.171 | 1.00 | 33.69 |
| ATOM | 4455 | CB  | ASP | B | 279 | 43.864 | 16.870 | 56.522 | 1.00 | 34.31 |
| ATOM | 4456 | CG  | ASP | B | 279 | 44.369 | 17.652 | 55.325 | 1.00 | 49.90 |
| ATOM | 4457 | OD1 | ASP | B | 279 | 45.255 | 17.163 | 54.584 | 1.00 | 38.05 |
| ATOM | 4458 | OD2 | ASP | B | 279 | 43.867 | 18.782 | 55.115 | 1.00 | 40.80 |
| ATOM | 4459 | C   | ASP | B | 279 | 45.697 | 16.716 | 58.238 | 1.00 | 26.60 |
| ATOM | 4460 | O   | ASP | B | 279 | 46.841 | 17.124 | 58.034 | 1.00 | 28.11 |
| ATOM | 4461 | N   | LEU | B | 280 | 45.088 | 16.895 | 59.408 | 1.00 | 25.81 |
| ATOM | 4462 | CA  | LEU | B | 280 | 45.801 | 17.538 | 60.510 | 1.00 | 28.08 |
| ATOM | 4463 | CB  | LEU | B | 280 | 44.955 | 17.535 | 61.782 | 1.00 | 24.40 |
| ATOM | 4464 | CG  | LEU | B | 280 | 43.689 | 18.389 | 61.749 | 1.00 | 26.95 |
| ATOM | 4465 | CD1 | LEU | B | 280 | 43.088 | 18.489 | 63.138 | 1.00 | 30.65 |
| ATOM | 4466 | CD2 | LEU | B | 280 | 43.987 | 19.757 | 61.164 | 1.00 | 49.17 |
| ATOM | 4467 | C   | LEU | B | 280 | 47.117 | 16.834 | 60.804 | 1.00 | 32.98 |
| ATOM | 4468 | O   | LEU | B | 280 | 48.141 | 17.483 | 61.022 | 1.00 | 28.16 |
| ATOM | 4469 | N   | ARG | B | 281 | 47.078 | 15.503 | 60.816 | 1.00 | 21.92 |
| ATOM | 4470 | CA  | ARG | B | 281 | 48.252 | 14.703 | 61.134 | 1.00 | 14.30 |
| ATOM | 4471 | CB  | ARG | B | 281 | 47.854 | 13.212 | 61.199 | 1.00 | 15.59 |

**FIGURE 188**



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4472 | CG  | ARG | B | 281 | 46.856 | 12.946 | 62.326 | 1.00 | 30.08 |
| ATOM | 4473 | CD  | ARG | B | 281 | 47.580 | 12.419 | 63.554 | 1.00 | 35.07 |
| ATOM | 4474 | NE  | ARG | B | 281 | 46.665 | 12.288 | 64.685 | 1.00 | 41.36 |
| ATOM | 4475 | CZ  | ARG | B | 281 | 46.356 | 11.125 | 65.243 | 1.00 | 44.73 |
| ATOM | 4476 | NH1 | ARG | B | 281 | 46.894 | 10.010 | 64.769 | 1.00 | 39.14 |
| ATOM | 4477 | NH2 | ARG | B | 281 | 45.515 | 11.092 | 66.268 | 1.00 | 40.94 |
| ATOM | 4478 | C   | ARG | B | 281 | 49.378 | 14.834 | 60.141 | 1.00 | 16.56 |
| ATOM | 4479 | O   | ARG | B | 281 | 50.574 | 14.692 | 60.430 | 1.00 | 23.41 |
| ATOM | 4480 | N   | LEU | B | 282 | 49.000 | 15.098 | 58.885 | 1.00 | 21.94 |
| ATOM | 4481 | CA  | LEU | B | 282 | 50.085 | 15.295 | 57.919 | 1.00 | 22.08 |
| ATOM | 4482 | CB  | LEU | B | 282 | 49.505 | 15.415 | 56.508 | 1.00 | 30.24 |
| ATOM | 4483 | CG  | LEU | B | 282 | 48.946 | 14.129 | 55.895 | 1.00 | 38.66 |
| ATOM | 4484 | CD1 | LEU | B | 282 | 48.260 | 14.402 | 54.563 | 1.00 | 35.05 |
| ATOM | 4485 | CD2 | LEU | B | 282 | 50.055 | 13.099 | 55.724 | 1.00 | 35.97 |
| ATOM | 4486 | C   | LEU | B | 282 | 50.921 | 16.528 | 58.246 | 1.00 | 22.11 |
| ATOM | 4487 | O   | LEU | B | 282 | 52.089 | 16.605 | 57.854 | 1.00 | 27.03 |
| ATOM | 4488 | N   | HIS | B | 283 | 50.359 | 17.509 | 58.949 | 1.00 | 19.17 |
| ATOM | 4489 | CA  | HIS | B | 283 | 51.085 | 18.767 | 59.129 | 1.00 | 22.40 |
| ATOM | 4490 | CB  | HIS | B | 283 | 50.140 | 19.931 | 58.762 | 1.00 | 28.15 |
| ATOM | 4491 | CG  | HIS | B | 283 | 49.775 | 19.824 | 57.305 | 1.00 | 27.86 |
| ATOM | 4492 | ND1 | HIS | B | 283 | 48.636 | 19.183 | 56.872 | 1.00 | 29.65 |
| ATOM | 4493 | CE1 | HIS | B | 283 | 48.585 | 19.229 | 55.549 | 1.00 | 28.25 |
| ATOM | 4494 | NE2 | HIS | B | 283 | 49.648 | 19.884 | 55.115 | 1.00 | 28.83 |
| ATOM | 4495 | CD2 | HIS | B | 283 | 50.417 | 20.257 | 56.193 | 1.00 | 25.31 |
| ATOM | 4496 | C   | HIS | B | 283 | 51.683 | 18.946 | 60.513 | 1.00 | 16.39 |
| ATOM | 4497 | O   | HIS | B | 283 | 52.619 | 19.732 | 60.696 | 1.00 | 19.23 |
| ATOM | 4498 | N   | ARG | B | 284 | 51.215 | 18.186 | 61.499 | 1.00 | 14.42 |
| ATOM | 4499 | CA  | ARG | B | 284 | 51.851 | 18.254 | 62.811 | 1.00 | 16.63 |
| ATOM | 4500 | CB  | ARG | B | 284 | 51.353 | 19.503 | 63.539 | 1.00 | 17.04 |
| ATOM | 4501 | CG  | ARG | B | 284 | 51.990 | 19.779 | 64.894 | 1.00 | 20.73 |
| ATOM | 4502 | CD  | ARG | B | 284 | 51.670 | 21.227 | 65.288 | 1.00 | 19.31 |
| ATOM | 4503 | NE  | ARG | B | 284 | 51.932 | 21.473 | 66.705 | 1.00 | 16.50 |
| ATOM | 4504 | CZ  | ARG | B | 284 | 53.027 | 22.065 | 67.155 | 1.00 | 18.89 |
| ATOM | 4505 | NH1 | ARG | B | 284 | 53.961 | 22.471 | 66.295 | 1.00 | 16.50 |
| ATOM | 4506 | NH2 | ARG | B | 284 | 53.184 | 22.249 | 68.464 | 1.00 | 12.75 |
| ATOM | 4507 | C   | ARG | B | 284 | 51.515 | 17.002 | 63.621 | 1.00 | 15.24 |
| ATOM | 4508 | O   | ARG | B | 284 | 50.395 | 16.503 | 63.515 | 1.00 | 21.78 |
| ATOM | 4509 | N   | VAL | B | 285 | 52.472 | 16.553 | 64.400 | 1.00 | 22.07 |
| ATOM | 4510 | CA  | VAL | B | 285 | 52.309 | 15.357 | 65.228 | 1.00 | 18.47 |
| ATOM | 4511 | CB  | VAL | B | 285 | 53.643 | 15.032 | 65.919 | 1.00 | 22.85 |
| ATOM | 4512 | CG1 | VAL | B | 285 | 53.931 | 15.996 | 67.065 | 1.00 | 21.98 |
| ATOM | 4513 | CG2 | VAL | B | 285 | 53.647 | 13.591 | 66.415 | 1.00 | 31.56 |
| ATOM | 4514 | C   | VAL | B | 285 | 51.181 | 15.513 | 66.237 | 1.00 | 31.62 |
| ATOM | 4515 | O   | VAL | B | 285 | 50.887 | 16.594 | 66.739 | 1.00 | 20.75 |
| ATOM | 4516 | N   | HIS | B | 286 | 50.511 | 14.404 | 66.519 | 1.00 | 35.82 |
| ATOM | 4517 | CA  | HIS | B | 286 | 49.576 | 14.183 | 67.598 | 1.00 | 24.99 |
| ATOM | 4518 | CB  | HIS | B | 286 | 50.264 | 14.498 | 68.941 | 1.00 | 23.90 |
| ATOM | 4519 | CG  | HIS | B | 286 | 51.337 | 13.511 | 69.289 | 1.00 | 30.81 |
| ATOM | 4520 | ND1 | HIS | B | 286 | 51.236 | 12.162 | 69.015 | 1.00 | 39.23 |
| ATOM | 4521 | CE1 | HIS | B | 286 | 52.326 | 11.537 | 69.425 | 1.00 | 40.25 |
| ATOM | 4522 | NE2 | HIS | B | 286 | 53.144 | 12.431 | 69.963 | 1.00 | 40.87 |
| ATOM | 4523 | CD2 | HIS | B | 286 | 52.543 | 13.669 | 69.883 | 1.00 | 30.11 |

**FIGURE 189**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|---|
| ATOM | 4524 | C   | HIS | B | 286 | 48.282 | 14.973 | 67.520 | 1.00 | 28.12  |   |
| ATOM | 4525 | O   | HIS | B | 286 | 47.543 | 15.026 | 68.515 | 1.00 | 34.48  |   |
| ATOM | 4526 | N   | MET | B | 287 | 47.981 | 15.578 | 66.382 | 1.00 | 19.24  |   |
| ATOM | 4527 | CA  | MET | B | 287 | 46.741 | 16.320 | 66.214 | 1.00 | 22.67  |   |
| ATOM | 4528 | CB  | MET | B | 287 | 46.545 | 16.759 | 64.771 | 1.00 | 29.06  |   |
| ATOM | 4529 | CG  | MET | B | 287 | 47.551 | 17.692 | 64.153 | 1.00 | 26.09  |   |
| ATOM | 4530 | SD  | MET | B | 287 | 47.319 | 19.403 | 64.727 | 1.00 | 57.61  | 1 |
| ATOM | 4531 | CE  | MET | B | 287 | 48.486 | 19.307 | 66.054 | 1.00 | 8.09   |   |
| ATOM | 4532 | C   | MET | B | 287 | 45.535 | 15.468 | 66.623 | 1.00 | 35.86  |   |
| ATOM | 4533 | O   | MET | B | 287 | 45.367 | 14.357 | 66.108 | 1.00 | 33.56  |   |
| ATOM | 4534 | N   | VAL | B | 288 | 44.728 | 16.000 | 67.527 | 1.00 | 31.94  |   |
| ATOM | 4535 | CA  | VAL | B | 288 | 43.671 | 15.249 | 68.206 | 1.00 | 29.58  |   |
| ATOM | 4536 | CB  | VAL | B | 288 | 42.591 | 14.724 | 67.262 | 1.00 | 25.44  |   |
| ATOM | 4537 | CG1 | VAL | B | 288 | 41.504 | 13.994 | 68.051 | 1.00 | 27.03  |   |
| ATOM | 4538 | CG2 | VAL | B | 288 | 41.978 | 15.870 | 66.483 | 1.00 | 25.23  |   |
| ATOM | 4539 | C   | VAL | B | 288 | 44.331 | 14.102 | 68.975 | 1.00 | 28.49  |   |
| ATOM | 4540 | O   | VAL | B | 288 | 44.486 | 12.998 | 68.463 | 1.00 | 31.96  |   |
| ATOM | 4541 | N   | GLN | B | 289 | 44.734 | 14.434 | 70.194 | 1.00 | 22.07  |   |
| ATOM | 4542 | CA  | GLN | B | 289 | 45.722 | 13.703 | 70.953 | 1.00 | 30.99  |   |
| ATOM | 4543 | CB  | GLN | B | 289 | 46.399 | 14.641 | 71.955 | 1.00 | 32.52  |   |
| ATOM | 4544 | CG  | GLN | B | 289 | 47.584 | 14.032 | 72.686 | 1.00 | 31.56  |   |
| ATOM | 4545 | CD  | GLN | B | 289 | 47.342 | 13.990 | 74.187 | 1.00 | 46.43  |   |
| ATOM | 4546 | OE1 | GLN | B | 289 | 46.897 | 14.972 | 74.782 | 1.00 | 45.11  |   |
| ATOM | 4547 | NE2 | GLN | B | 289 | 47.639 | 12.848 | 74.795 | 1.00 | 56.32  |   |
| ATOM | 4548 | C   | GLN | B | 289 | 45.165 | 12.495 | 71.695 | 1.00 | 34.06  |   |
| ATOM | 4549 | O   | GLN | B | 289 | 45.949 | 11.582 | 71.976 | 1.00 | 37.74  |   |
| ATOM | 4550 | N   | THR | B | 290 | 43.874 | 12.473 | 71.997 | 1.00 | 34.47  |   |
| ATOM | 4551 | CA  | THR | B | 290 | 43.323 | 11.278 | 72.636 | 1.00 | 38.23  |   |
| ATOM | 4552 | CB  | THR | B | 290 | 42.869 | 11.533 | 74.089 | 1.00 | 29.88  |   |
| ATOM | 4553 | OG1 | THR | B | 290 | 41.723 | 12.396 | 74.064 | 1.00 | 32.43  |   |
| ATOM | 4554 | CG2 | THR | B | 290 | 43.954 | 12.209 | 74.903 | 1.00 | 30.96  |   |
| ATOM | 4555 | C   | THR | B | 290 | 42.131 | 10.704 | 71.879 | 1.00 | 38.89  |   |
| ATOM | 4556 | O   | THR | B | 290 | 41.394 | 11.381 | 71.170 | 1.00 | 37.95  |   |
| ATOM | 4557 | N   | GLU | B | 291 | 41.927 | 9.397  | 72.062 | 1.00 | 40.68  |   |
| ATOM | 4558 | CA  | GLU | B | 291 | 40.760 | 8.735  | 71.494 | 1.00 | 35.35  |   |
| ATOM | 4559 | CB  | GLU | B | 291 | 40.764 | 7.261  | 71.915 | 1.00 | 46.96  |   |
| ATOM | 4560 | CG  | GLU | B | 291 | 39.750 | 6.391  | 71.186 | 1.00 | 52.82  |   |
| ATOM | 4561 | CD  | GLU | B | 291 | 39.890 | 4.935  | 71.603 | 1.00 | 55.59  |   |
| ATOM | 4562 | OE1 | GLU | B | 291 | 38.878 | 4.210  | 71.644 | 1.00 | 67.94  |   |
| ATOM | 4563 | OE2 | GLU | B | 291 | 41.035 | 4.536  | 71.899 | 1.00 | 48.99  |   |
| ATOM | 4564 | C   | GLU | B | 291 | 39.465 | 9.394  | 71.939 | 1.00 | 29.83  |   |
| ATOM | 4565 | O   | GLU | B | 291 | 38.487 | 9.486  | 71.192 | 1.00 | 34.01  |   |
| ATOM | 4566 | N   | CYS | B | 292 | 39.421 | 9.874  | 73.194 | 1.00 | 31.22  |   |
| ATOM | 4567 | CA  | CYS | B | 292 | 38.144 | 10.429 | 73.647 | 1.00 | 30.43  |   |
| ATOM | 4568 | CB  | CYS | B | 292 | 38.112 | 10.562 | 75.169 | 1.00 | 36.01  |   |
| ATOM | 4569 | SG  | CYS | B | 292 | 39.681 | 11.083 | 75.904 | 1.00 | 131.76 | 1 |
| ATOM | 4570 | C   | CYS | B | 292 | 37.862 | 11.764 | 72.979 | 1.00 | 24.32  |   |
| ATOM | 4571 | O   | CYS | B | 292 | 36.720 | 12.200 | 72.903 | 1.00 | 28.29  |   |
| ATOM | 4572 | N   | GLN | B | 293 | 38.915 | 12.415 | 72.489 | 1.00 | 33.10  |   |
| ATOM | 4573 | CA  | GLN | B | 293 | 38.751 | 13.630 | 71.694 | 1.00 | 30.62  |   |
| ATOM | 4574 | CB  | GLN | B | 293 | 40.117 | 14.322 | 71.527 | 1.00 | 28.49  |   |
| ATOM | 4575 | CG  | GLN | B | 293 | 40.470 | 15.209 | 72.711 | 1.00 | 27.02  |   |

**FIGURE 190**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 4576 | CD  | GLN | B | 293 | 41.904 | 15.666 | 72.787 | 1.00 | 29.40 |
| ATOM | 4577 | OE1 | GLN | B | 293 | 42.722 | 15.395 | 71.907 | 1.00 | 31.27 |
| ATOM | 4578 | NE2 | GLN | B | 293 | 42.261 | 16.375 | 73.858 | 1.00 | 29.27 |
| ATOM | 4579 | C   | GLN | B | 293 | 38.132 | 13.286 | 70.347 | 1.00 | 26.72 |
| ATOM | 4580 | O   | GLN | B | 293 | 37.224 | 13.930 | 69.828 | 1.00 | 39.00 |
| ATOM | 4581 | N   | TYR | B | 294 | 38.662 | 12.203 | 69.763 | 1.00 | 28.45 |
| ATOM | 4582 | CA  | TYR | B | 294 | 38.117 | 11.677 | 68.512 | 1.00 | 24.87 |
| ATOM | 4583 | CB  | TYR | B | 294 | 38.861 | 10.398 | 68.098 | 1.00 | 32.22 |
| ATOM | 4584 | CG  | TYR | B | 294 | 38.628 | 10.021 | 66.650 | 1.00 | 42.38 |
| ATOM | 4585 | CD1 | TYR | B | 294 | 39.072 | 10.848 | 65.621 | 1.00 | 43.00 |
| ATOM | 4586 | CE1 | TYR | B | 294 | 38.867 | 10.520 | 64.294 | 1.00 | 47.37 |
| ATOM | 4587 | CZ  | TYR | B | 294 | 38.207 | 9.350  | 63.975 | 1.00 | 48.16 |
| ATOM | 4588 | OH  | TYR | B | 294 | 38.001 | 9.025  | 62.651 | 1.00 | 34.98 |
| ATOM | 4589 | CE2 | TYR | B | 294 | 37.756 | 8.516  | 64.976 | 1.00 | 41.30 |
| ATOM | 4590 | CD2 | TYR | B | 294 | 37.966 | 8.851  | 66.302 | 1.00 | 40.38 |
| ATOM | 4591 | C   | TYR | B | 294 | 36.628 | 11.405 | 68.664 | 1.00 | 32.24 |
| ATOM | 4592 | O   | TYR | B | 294 | 35.800 | 11.862 | 67.885 | 1.00 | 38.08 |
| ATOM | 4593 | N   | VAL | B | 295 | 36.302 | 10.647 | 69.711 | 1.00 | 45.53 |
| ATOM | 4594 | CA  | VAL | B | 295 | 34.926 | 10.315 | 70.045 | 1.00 | 44.59 |
| ATOM | 4595 | CB  | VAL | B | 295 | 34.844 | 9.467  | 71.331 | 1.00 | 40.45 |
| ATOM | 4596 | CG1 | VAL | B | 295 | 33.478 | 9.640  | 71.975 | 1.00 | 39.76 |
| ATOM | 4597 | CG2 | VAL | B | 295 | 35.134 | 8.009  | 71.030 | 1.00 | 42.13 |
| ATOM | 4598 | C   | VAL | B | 295 | 34.096 | 11.573 | 70.258 | 1.00 | 43.22 |
| ATOM | 4599 | O   | VAL | B | 295 | 32.963 | 11.696 | 69.798 | 1.00 | 39.21 |
| ATOM | 4600 | N   | TYR | B | 296 | 34.680 | 12.529 | 70.983 | 1.00 | 39.28 |
| ATOM | 4601 | CA  | TYR | B | 296 | 33.973 | 13.791 | 71.204 | 1.00 | 38.11 |
| ATOM | 4602 | CB  | TYR | B | 296 | 34.866 | 14.740 | 72.004 | 1.00 | 36.49 |
| ATOM | 4603 | CG  | TYR | B | 296 | 34.235 | 16.065 | 72.341 | 1.00 | 29.43 |
| ATOM | 4604 | CD1 | TYR | B | 296 | 33.274 | 16.182 | 73.337 | 1.00 | 26.96 |
| ATOM | 4605 | CE1 | TYR | B | 296 | 32.688 | 17.392 | 73.655 | 1.00 | 26.29 |
| ATOM | 4606 | CZ  | TYR | B | 296 | 33.072 | 18.524 | 72.963 | 1.00 | 36.48 |
| ATOM | 4607 | OH  | TYR | B | 296 | 32.503 | 19.739 | 73.267 | 1.00 | 28.44 |
| ATOM | 4608 | CE2 | TYR | B | 296 | 34.023 | 18.443 | 71.970 | 1.00 | 34.08 |
| ATOM | 4609 | CD2 | TYR | B | 296 | 34.602 | 17.224 | 71.661 | 1.00 | 38.40 |
| ATOM | 4610 | C   | TYR | B | 296 | 33.582 | 14.431 | 69.883 | 1.00 | 30.28 |
| ATOM | 4611 | O   | TYR | B | 296 | 32.516 | 15.027 | 69.739 | 1.00 | 28.21 |
| ATOM | 4612 | N   | LEU | B | 297 | 34.477 | 14.309 | 68.896 | 1.00 | 32.45 |
| ATOM | 4613 | CA  | LEU | B | 297 | 34.172 | 14.905 | 67.592 | 1.00 | 29.13 |
| ATOM | 4614 | CB  | LEU | B | 297 | 35.329 | 14.627 | 66.633 | 1.00 | 28.47 |
| ATOM | 4615 | CG  | LEU | B | 297 | 36.560 | 15.523 | 66.842 | 1.00 | 31.47 |
| ATOM | 4616 | CD1 | LEU | B | 297 | 37.742 | 14.998 | 66.052 | 1.00 | 24.45 |
| ATOM | 4617 | CD2 | LEU | B | 297 | 36.235 | 16.958 | 66.462 | 1.00 | 26.38 |
| ATOM | 4618 | C   | LEU | B | 297 | 32.852 | 14.378 | 67.039 | 1.00 | 34.78 |
| ATOM | 4619 | O   | LEU | B | 297 | 31.967 | 15.133 | 66.639 | 1.00 | 26.92 |
| ATOM | 4620 | N   | HIS | B | 298 | 32.719 | 13.055 | 67.036 | 1.00 | 42.39 |
| ATOM | 4621 | CA  | HIS | B | 298 | 31.505 | 12.405 | 66.536 | 1.00 | 42.94 |
| ATOM | 4622 | CB  | HIS | B | 298 | 31.714 | 10.888 | 66.528 | 1.00 | 40.75 |
| ATOM | 4623 | CG  | HIS | B | 298 | 32.747 | 10.427 | 65.545 | 1.00 | 42.36 |
| ATOM | 4624 | ND1 | HIS | B | 298 | 34.085 | 10.309 | 65.850 | 1.00 | 43.84 |
| ATOM | 4625 | CE1 | HIS | B | 298 | 34.758 | 9.881  | 64.795 | 1.00 | 39.31 |
| ATOM | 4626 | NE2 | HIS | B | 298 | 33.901 | 9.708  | 63.804 | 1.00 | 42.05 |
| ATOM | 4627 | CD2 | HIS | B | 298 | 32.640 | 10.043 | 64.249 | 1.00 | 43.47 |

**FIGURE 191**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |   |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|---|
| ATOM | 4628 | C   | HIS | B | 298 | 30.278 | 12.791 | 67.348 | 1.00 | 35.51 |   |
| ATOM | 4629 | O   | HIS | B | 298 | 29.192 | 12.997 | 66.800 | 1.00 | 32.51 |   |
| ATOM | 4630 | N   | GLN | B | 299 | 30.409 | 12.916 | 68.669 | 1.00 | 33.21 |   |
| ATOM | 4631 | CA  | GLN | B | 299 | 29.266 | 13.336 | 69.483 | 1.00 | 33.23 |   |
| ATOM | 4632 | CB  | GLN | B | 299 | 29.581 | 13.264 | 70.982 | 1.00 | 40.20 |   |
| ATOM | 4633 | CG  | GLN | B | 299 | 30.119 | 11.919 | 71.443 | 1.00 | 49.41 |   |
| ATOM | 4634 | CD  | GLN | B | 299 | 30.348 | 11.829 | 72.937 | 1.00 | 54.91 |   |
| ATOM | 4635 | OE1 | GLN | B | 299 | 31.345 | 12.313 | 73.477 | 1.00 | 54.96 |   |
| ATOM | 4636 | NE2 | GLN | B | 299 | 29.412 | 11.192 | 73.633 | 1.00 | 62.12 |   |
| ATOM | 4637 | C   | GLN | B | 299 | 28.826 | 14.743 | 69.114 | 1.00 | 32.95 |   |
| ATOM | 4638 | O   | GLN | B | 299 | 27.638 | 15.068 | 69.089 | 1.00 | 41.61 |   |
| ATOM | 4639 | N   | CYS | B | 300 | 29.787 | 15.623 | 68.810 | 1.00 | 32.51 |   |
| ATOM | 4640 | CA  | CYS | B | 300 | 29.370 | 16.967 | 68.419 | 1.00 | 25.41 |   |
| ATOM | 4641 | CB  | CYS | B | 300 | 30.603 | 17.848 | 68.163 | 1.00 | 23.71 |   |
| ATOM | 4642 | SG  | CYS | B | 300 | 31.486 | 18.320 | 69.679 | 1.00 | 41.45 | 1 |
| ATOM | 4643 | C   | CYS | B | 300 | 28.493 | 16.946 | 67.175 | 1.00 | 29.79 |   |
| ATOM | 4644 | O   | CYS | B | 300 | 27.472 | 17.628 | 67.074 | 1.00 | 30.90 |   |
| ATOM | 4645 | N   | VAL | B | 301 | 28.920 | 16.157 | 66.190 | 1.00 | 37.78 |   |
| ATOM | 4646 | CA  | VAL | B | 301 | 28.176 | 16.043 | 64.943 | 1.00 | 31.92 |   |
| ATOM | 4647 | CB  | VAL | B | 301 | 28.938 | 15.212 | 63.899 | 1.00 | 35.00 |   |
| ATOM | 4648 | CG1 | VAL | B | 301 | 28.024 | 14.868 | 62.728 | 1.00 | 40.94 |   |
| ATOM | 4649 | CG2 | VAL | B | 301 | 30.179 | 15.957 | 63.430 | 1.00 | 37.17 |   |
| ATOM | 4650 | C   | VAL | B | 301 | 26.819 | 15.404 | 65.220 | 1.00 | 27.85 |   |
| ATOM | 4651 | O   | VAL | B | 301 | 25.795 | 15.854 | 64.720 | 1.00 | 36.79 |   |
| ATOM | 4652 | N   | ARG | B | 302 | 26.825 | 14.349 | 66.036 | 1.00 | 42.30 |   |
| ATOM | 4653 | CA  | ARG | B | 302 | 25.557 | 13.697 | 66.370 | 1.00 | 48.19 |   |
| ATOM | 4654 | CB  | ARG | B | 302 | 25.771 | 12.523 | 67.322 | 1.00 | 48.82 |   |
| ATOM | 4655 | CG  | ARG | B | 302 | 24.477 | 11.943 | 67.886 | 1.00 | 51.72 |   |
| ATOM | 4656 | CD  | ARG | B | 302 | 24.723 | 11.322 | 69.253 | 1.00 | 57.09 |   |
| ATOM | 4657 | NE  | ARG | B | 302 | 24.895 | 12.340 | 70.291 | 1.00 | 63.02 |   |
| ATOM | 4658 | CZ  | ARG | B | 302 | 25.940 | 12.384 | 71.110 | 1.00 | 68.57 |   |
| ATOM | 4659 | NH1 | ARG | B | 302 | 26.895 | 11.472 | 71.013 | 1.00 | 88.06 |   |
| ATOM | 4660 | NH2 | ARG | B | 302 | 26.046 | 13.329 | 72.036 | 1.00 | 62.92 |   |
| ATOM | 4661 | C   | ARG | B | 302 | 24.599 | 14.715 | 66.979 | 1.00 | 52.02 |   |
| ATOM | 4662 | O   | ARG | B | 302 | 23.481 | 14.911 | 66.506 | 1.00 | 55.97 |   |
| ATOM | 4663 | N   | ASP | B | 303 | 25.064 | 15.381 | 68.036 | 1.00 | 43.78 |   |
| ATOM | 4664 | CA  | ASP | B | 303 | 24.206 | 16.380 | 68.673 | 1.00 | 41.33 |   |
| ATOM | 4665 | CB  | ASP | B | 303 | 24.923 | 16.943 | 69.911 | 1.00 | 45.65 |   |
| ATOM | 4666 | CG  | ASP | B | 303 | 25.039 | 15.864 | 70.980 | 1.00 | 50.16 |   |
| ATOM | 4667 | OD1 | ASP | B | 303 | 24.298 | 14.861 | 70.855 | 1.00 | 45.98 |   |
| ATOM | 4668 | OD2 | ASP | B | 303 | 25.846 | 15.982 | 71.927 | 1.00 | 34.68 |   |
| ATOM | 4669 | C   | ASP | B | 303 | 23.795 | 17.459 | 67.691 | 1.00 | 40.46 |   |
| ATOM | 4670 | O   | ASP | B | 303 | 22.662 | 17.955 | 67.734 | 1.00 | 56.09 |   |
| ATOM | 4671 | N   | VAL | B | 304 | 24.662 | 17.874 | 66.763 | 1.00 | 34.45 |   |
| ATOM | 4672 | CA  | VAL | B | 304 | 24.201 | 18.942 | 65.868 | 1.00 | 48.95 |   |
| ATOM | 4673 | CB  | VAL | B | 304 | 25.351 | 19.587 | 65.075 | 1.00 | 49.79 |   |
| ATOM | 4674 | CG1 | VAL | B | 304 | 24.862 | 20.185 | 63.765 | 1.00 | 28.51 |   |
| ATOM | 4675 | CG2 | VAL | B | 304 | 26.027 | 20.662 | 65.919 | 1.00 | 59.44 |   |
| ATOM | 4676 | C   | VAL | B | 304 | 23.143 | 18.410 | 64.907 | 1.00 | 54.85 |   |
| ATOM | 4677 | O   | VAL | B | 304 | 22.147 | 19.072 | 64.611 | 1.00 | 47.47 |   |
| ATOM | 4678 | N   | LEU | B | 305 | 23.356 | 17.194 | 64.408 | 1.00 | 51.63 |   |
| ATOM | 4679 | CA  | LEU | B | 305 | 22.375 | 16.636 | 63.478 | 1.00 | 51.67 |   |

**FIGURE 192**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |        |
|------|------|-----|-----|---|-----|--------|--------|--------|------|--------|
| ATOM | 4680 | CB  | LEU | B | 305 | 22.844 | 15.260 | 62.996 | 1.00 | 41.22  |
| ATOM | 4681 | CG  | LEU | B | 305 | 24.018 | 15.265 | 62.015 | 1.00 | 34.32  |
| ATOM | 4682 | CD1 | LEU | B | 305 | 24.215 | 13.904 | 61.375 | 1.00 | 47.80  |
| ATOM | 4683 | CD2 | LEU | B | 305 | 23.809 | 16.325 | 60.944 | 1.00 | 28.65  |
| ATOM | 4684 | C   | LEU | B | 305 | 21.001 | 16.567 | 64.128 | 1.00 | 56.67  |
| ATOM | 4685 | O   | LEU | B | 305 | 20.041 | 17.177 | 63.650 | 1.00 | 54.42  |
| ATOM | 4686 | N   | ARG | B | 306 | 20.874 | 15.835 | 65.235 | 1.00 | 57.52  |
| ATOM | 4687 | CA  | ARG | B | 306 | 19.539 | 15.658 | 65.806 | 1.00 | 66.45  |
| ATOM | 4688 | CB  | ARG | B | 306 | 19.575 | 14.723 | 67.019 | 1.00 | 67.88  |
| ATOM | 4689 | CG  | ARG | B | 306 | 20.951 | 14.533 | 67.625 | 1.00 | 72.91  |
| ATOM | 4690 | CD  | ARG | B | 306 | 20.877 | 14.354 | 69.133 | 1.00 | 75.55  |
| ATOM | 4691 | NE  | ARG | B | 306 | 21.300 | 13.007 | 69.521 | 1.00 | 78.32  |
| ATOM | 4692 | CZ  | ARG | B | 306 | 21.914 | 12.752 | 70.670 | 1.00 | 79.74  |
| ATOM | 4693 | NH1 | ARG | B | 306 | 22.161 | 13.748 | 71.509 | 1.00 | 73.02  |
| ATOM | 4694 | NH2 | ARG | B | 306 | 22.275 | 11.514 | 70.971 | 1.00 | 90.52  |
| ATOM | 4695 | C   | ARG | B | 306 | 18.884 | 16.972 | 66.211 | 1.00 | 65.71  |
| ATOM | 4696 | O   | ARG | B | 306 | 17.651 | 17.050 | 66.270 | 1.00 | 60.57  |
| ATOM | 4697 | N   | ALA | B | 307 | 19.674 | 18.000 | 66.503 | 1.00 | 63.41  |
| ATOM | 4698 | CA  | ALA | B | 307 | 19.082 | 19.268 | 66.929 | 1.00 | 60.95  |
| ATOM | 4699 | CB  | ALA | B | 307 | 20.137 | 20.143 | 67.585 | 1.00 | 47.72  |
| ATOM | 4700 | C   | ALA | B | 307 | 18.413 | 19.987 | 65.760 | 1.00 | 65.50  |
| ATOM | 4701 | O   | ALA | B | 307 | 17.285 | 20.470 | 65.877 | 1.00 | 57.65  |
| ATOM | 4702 | N   | ARG | B | 308 | 19.113 | 20.054 | 64.634 | 1.00 | 73.88  |
| ATOM | 4703 | CA  | ARG | B | 308 | 18.601 | 20.681 | 63.421 | 1.00 | 83.95  |
| ATOM | 4704 | CB  | ARG | B | 308 | 19.685 | 20.718 | 62.342 | 1.00 | 82.20  |
| ATOM | 4705 | CG  | ARG | B | 308 | 21.069 | 21.087 | 62.860 | 1.00 | 81.07  |
| ATOM | 4706 | CD  | ARG | B | 308 | 22.138 | 20.840 | 61.803 | 1.00 | 76.97  |
| ATOM | 4707 | NE  | ARG | B | 308 | 21.546 | 20.677 | 60.482 | 1.00 | 76.87  |
| ATOM | 4708 | CZ  | ARG | B | 308 | 22.159 | 20.442 | 59.337 | 1.00 | 74.18  |
| ATOM | 4709 | NH1 | ARG | B | 308 | 23.476 | 20.316 | 59.248 | 1.00 | 57.78  |
| ATOM | 4710 | NH2 | ARG | B | 308 | 21.427 | 20.324 | 58.233 | 1.00 | 64.71  |
| ATOM | 4711 | C   | ARG | B | 308 | 17.365 | 19.943 | 62.917 | 1.00 | 92.86  |
| ATOM | 4712 | O   | ARG | B | 308 | 16.278 | 20.515 | 62.815 | 1.00 | 85.75  |
| ATOM | 4713 | N   | LYS | B | 309 | 17.535 | 18.658 | 62.606 | 1.00 | 97.18  |
| ATOM | 4714 | CA  | LYS | B | 309 | 16.407 | 17.851 | 62.152 | 1.00 | 101.48 |
| ATOM | 4715 | CB  | LYS | B | 309 | 16.828 | 16.414 | 61.850 | 1.00 | 103.32 |
| ATOM | 4716 | CG  | LYS | B | 309 | 15.687 | 15.410 | 61.805 | 1.00 | 104.02 |
| ATOM | 4717 | CD  | LYS | B | 309 | 15.273 | 15.077 | 60.382 | 1.00 | 104.29 |
| ATOM | 4718 | CE  | LYS | B | 309 | 13.920 | 14.382 | 60.342 | 1.00 | 101.24 |
| ATOM | 4719 | NZ  | LYS | B | 309 | 13.811 | 13.409 | 59.216 | 1.00 | 84.67  |
| ATOM | 4720 | C   | LYS | B | 309 | 15.292 | 17.866 | 63.202 | 1.00 | 101.41 |
| ATOM | 4721 | O   | LYS | B | 309 | 15.282 | 16.996 | 64.071 | 1.00 | 109.20 |
| ATOM | 4722 | N   | LEU | B | 310 | 14.415 | 18.846 | 63.079 | 1.00 | 97.60  |
| ATOM | 4723 | CA  | LEU | B | 310 | 13.251 | 19.077 | 63.916 | 1.00 | 95.62  |
| ATOM | 4724 | CB  | LEU | B | 310 | 13.533 | 18.739 | 65.380 | 1.00 | 95.83  |
| ATOM | 4725 | CG  | LEU | B | 310 | 13.082 | 17.359 | 65.866 | 1.00 | 98.74  |
| ATOM | 4726 | CD1 | LEU | B | 310 | 12.607 | 16.487 | 64.713 | 1.00 | 84.93  |
| ATOM | 4727 | CD2 | LEU | B | 310 | 14.202 | 16.667 | 66.632 | 1.00 | 113.56 |
| ATOM | 4728 | C   | LEU | B | 310 | 12.786 | 20.528 | 63.789 | 1.00 | 92.71  |
| ATOM | 4729 | O   | LEU | B | 310 | 12.515 | 21.222 | 64.765 | 1.00 | 74.63  |
| ATOM | 4730 | O14 | INH | Z | 2   | 55.288 | 16.173 | 78.572 | 1.00 | 68.22  |
| ATOM | 4731 | O4  | INH | Z | 2   | 48.070 | 20.932 | 75.258 | 1.00 | 24.37  |

**FIGURE 193**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |   |        |        |        |      |       |   |
|------|------|-----|-----|---|---|--------|--------|--------|------|-------|---|
| ATOM | 4732 | S1  | INH | Z | 2 | 47.385 | 19.830 | 74.500 | 1.00 | 29.84 | 1 |
| ATOM | 4733 | O2  | INH | Z | 2 | 48.097 | 19.600 | 73.249 | 1.00 | 23.28 |   |
| ATOM | 4734 | O3  | INH | Z | 2 | 45.976 | 19.785 | 74.420 | 1.00 | 19.75 |   |
| ATOM | 4735 | N1  | INH | Z | 2 | 47.628 | 18.601 | 75.423 | 1.00 | 29.61 |   |
| ATOM | 4736 | C2  | INH | Z | 2 | 48.913 | 18.097 | 75.576 | 1.00 | 22.41 |   |
| ATOM | 4737 | C1  | INH | Z | 2 | 49.706 | 18.569 | 76.616 | 1.00 | 17.58 |   |
| ATOM | 4738 | C3  | INH | Z | 2 | 49.439 | 17.157 | 74.694 | 1.00 | 25.75 |   |
| ATOM | 4739 | C4  | INH | Z | 2 | 50.726 | 16.698 | 74.879 | 1.00 | 21.37 |   |
| ATOM | 4740 | C5  | INH | Z | 2 | 51.537 | 17.205 | 75.894 | 1.00 | 28.97 |   |
| ATOM | 4741 | C6  | INH | Z | 2 | 50.996 | 18.159 | 76.786 | 1.00 | 18.78 |   |
| ATOM | 4742 | C8  | INH | Z | 2 | 52.976 | 16.759 | 76.061 | 1.00 | 30.10 |   |
| ATOM | 4743 | C7  | INH | Z | 2 | 53.147 | 15.585 | 77.076 | 1.00 | 38.47 |   |
| ATOM | 4744 | C9  | INH | Z | 2 | 52.112 | 14.479 | 76.942 | 1.00 | 50.15 |   |
| ATOM | 4745 | N2  | INH | Z | 2 | 52.210 | 13.593 | 75.955 | 1.00 | 46.78 |   |
| ATOM | 4746 | C10 | INH | Z | 2 | 51.114 | 12.942 | 75.276 | 1.00 | 48.01 |   |
| ATOM | 4747 | O1  | INH | Z | 2 | 51.204 | 14.431 | 77.757 | 1.00 | 53.75 |   |
| ATOM | 4748 | N11 | INH | Z | 2 | 53.037 | 16.040 | 78.545 | 1.00 | 43.33 |   |
| ATOM | 4749 | C12 | INH | Z | 2 | 54.320 | 16.516 | 79.194 | 1.00 | 55.88 |   |
| ATOM | 4750 | O6  | INH | Z | 2 | 54.055 | 17.245 | 80.374 | 1.00 | 62.18 |   |
| ATOM | 4751 | C13 | INH | Z | 2 | 55.182 | 17.437 | 81.254 | 1.00 | 68.88 |   |
| ATOM | 4752 | C14 | INH | Z | 2 | 55.890 | 18.762 | 81.044 | 1.00 | 69.79 |   |
| ATOM | 4753 | C15 | INH | Z | 2 | 57.051 | 18.833 | 80.275 | 1.00 | 67.74 |   |
| ATOM | 4754 | C16 | INH | Z | 2 | 57.681 | 20.064 | 80.042 | 1.00 | 70.03 |   |
| ATOM | 4755 | C17 | INH | Z | 2 | 57.152 | 21.249 | 80.558 | 1.00 | 70.11 |   |
| ATOM | 4756 | C18 | INH | Z | 2 | 55.999 | 21.166 | 81.352 | 1.00 | 69.36 |   |
| ATOM | 4757 | C19 | INH | Z | 2 | 55.377 | 19.934 | 81.606 | 1.00 | 69.79 |   |
| ATOM | 4758 | O14 | INH | Z | 1 | -1.113 | 8.871  | 44.215 | 1.00 | 38.80 |   |
| ATOM | 4759 | O4  | INH | Z | 1 | 6.622  | 4.171  | 41.248 | 1.00 | 25.08 |   |
| ATOM | 4760 | S1  | INH | Z | 1 | 7.335  | 5.325  | 40.618 | 1.00 | 22.22 | 1 |
| ATOM | 4761 | O2  | INH | Z | 1 | 6.828  | 5.548  | 39.260 | 1.00 | 16.51 |   |
| ATOM | 4762 | O3  | INH | Z | 1 | 8.747  | 5.431  | 40.711 | 1.00 | 19.75 |   |
| ATOM | 4763 | N1  | INH | Z | 1 | 6.835  | 6.493  | 41.497 | 1.00 | 20.76 |   |
| ATOM | 4764 | C2  | INH | Z | 1 | 5.527  | 6.957  | 41.421 | 1.00 | 21.28 |   |
| ATOM | 4765 | C1  | INH | Z | 1 | 4.584  | 6.427  | 42.291 | 1.00 | 13.44 |   |
| ATOM | 4766 | C3  | INH | Z | 1 | 5.132  | 7.960  | 40.530 | 1.00 | 21.95 |   |
| ATOM | 4767 | C4  | INH | Z | 1 | 3.817  | 8.382  | 40.524 | 1.00 | 18.36 |   |
| ATOM | 4768 | C5  | INH | Z | 1 | 2.870  | 7.861  | 41.415 | 1.00 | 23.03 |   |
| ATOM | 4769 | C6  | INH | Z | 1 | 3.283  | 6.862  | 42.323 | 1.00 | 16.81 |   |
| ATOM | 4770 | C8  | INH | Z | 1 | 1.429  | 8.323  | 41.430 | 1.00 | 24.83 |   |
| ATOM | 4771 | C7  | INH | Z | 1 | 1.120  | 9.380  | 42.549 | 1.00 | 39.39 |   |
| ATOM | 4772 | C9  | INH | Z | 1 | 2.120  | 10.521 | 42.630 | 1.00 | 40.58 |   |
| ATOM | 4773 | N2  | INH | Z | 1 | 2.202  | 11.436 | 41.667 | 1.00 | 41.79 |   |
| ATOM | 4774 | C10 | INH | Z | 1 | 3.287  | 12.393 | 41.566 | 1.00 | 43.35 |   |
| ATOM | 4775 | O1  | INH | Z | 1 | 2.868  | 10.605 | 43.592 | 1.00 | 44.71 |   |
| ATOM | 4776 | N11 | INH | Z | 1 | 1.157  | 8.742  | 43.948 | 1.00 | 50.75 |   |
| ATOM | 4777 | C12 | INH | Z | 1 | -0.086 | 8.670  | 44.797 | 1.00 | 50.71 |   |
| ATOM | 4778 | O6  | INH | Z | 1 | 0.284  | 8.365  | 46.128 | 1.00 | 57.94 |   |
| ATOM | 4779 | C13 | INH | Z | 1 | -0.788 | 8.005  | 47.016 | 1.00 | 62.79 |   |
| ATOM | 4780 | C14 | INH | Z | 1 | -1.038 | 6.513  | 47.116 | 1.00 | 58.14 |   |
| ATOM | 4781 | C15 | INH | Z | 1 | -2.097 | 5.926  | 46.420 | 1.00 | 57.59 |   |
| ATOM | 4782 | C16 | INH | Z | 1 | -2.357 | 4.551  | 46.525 | 1.00 | 58.75 |   |
| ATOM | 4783 | C17 | INH | Z | 1 | -1.560 | 3.742  | 47.338 | 1.00 | 55.57 |   |

**FIGURE 194**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |    |        |         |        |      |       |
|------|------|-----|-----|---|----|--------|---------|--------|------|-------|
| ATOM | 4784 | C18 | INH | Z | 1  | -0.493 | 4.337   | 48.028 | 1.00 | 55.37 |
| ATOM | 4785 | C19 | INH | Z | 1  | -0.220 | 5.707   | 47.913 | 1.00 | 55.41 |
| ATOM | 4786 | O1  | HOH | W | 1  | 10.045 | -6.206  | 48.501 | 1.00 | 9.70  |
| ATOM | 4787 | O1  | HOH | W | 2  | 44.009 | 31.332  | 82.099 | 1.00 | 12.76 |
| ATOM | 4788 | O1  | HOH | W | 3  | -1.504 | 3.025   | 37.601 | 1.00 | 14.12 |
| ATOM | 4789 | O1  | HOH | W | 4  | 56.634 | 21.887  | 72.619 | 1.00 | 18.84 |
| ATOM | 4790 | O1  | HOH | W | 5  | -3.336 | -2.466  | 27.653 | 1.00 | 16.96 |
| ATOM | 4791 | O1  | HOH | W | 6  | 59.893 | 27.230  | 63.111 | 1.00 | 20.75 |
| ATOM | 4792 | O1  | HOH | W | 7  | 0.940  | 7.097   | 29.426 | 1.00 | 15.51 |
| ATOM | 4793 | O1  | HOH | W | 8  | 56.585 | 29.393  | 71.563 | 1.00 | 17.34 |
| ATOM | 4794 | O1  | HOH | W | 9  | -3.244 | -3.725  | 34.798 | 1.00 | 13.56 |
| ATOM | 4795 | O1  | HOH | W | 10 | 1.553  | -4.822  | 35.953 | 1.00 | 13.15 |
| ATOM | 4796 | O1  | HOH | W | 11 | -4.895 | -5.747  | 33.816 | 1.00 | 16.00 |
| ATOM | 4797 | O1  | HOH | W | 12 | 55.065 | 17.796  | 64.150 | 1.00 | 18.78 |
| ATOM | 4798 | O1  | HOH | W | 13 | -2.710 | 7.632   | 22.526 | 1.00 | 25.85 |
| ATOM | 4799 | O1  | HOH | W | 14 | -1.058 | -4.632  | 36.416 | 1.00 | 16.59 |
| ATOM | 4800 | O1  | HOH | W | 15 | 58.883 | 28.512  | 70.102 | 1.00 | 17.41 |
| ATOM | 4801 | O1  | HOH | W | 16 | 14.129 | -11.346 | 42.224 | 1.00 | 25.25 |
| ATOM | 4802 | O1  | HOH | W | 17 | 15.198 | -5.722  | 25.861 | 1.00 | 17.95 |
| ATOM | 4803 | O1  | HOH | W | 18 | -5.309 | 3.570   | 27.477 | 1.00 | 17.89 |
| ATOM | 4804 | O1  | HOH | W | 19 | 59.756 | 17.517  | 57.776 | 1.00 | 24.77 |
| ATOM | 4805 | O1  | HOH | W | 20 | -6.619 | -5.980  | 43.124 | 1.00 | 18.09 |
| ATOM | 4806 | O1  | HOH | W | 21 | 54.142 | 29.809  | 70.726 | 1.00 | 17.84 |
| ATOM | 4807 | O1  | HOH | W | 22 | 0.201  | -5.367  | 22.242 | 1.00 | 20.61 |
| ATOM | 4808 | O1  | HOH | W | 23 | 4.276  | 11.648  | 28.034 | 1.00 | 21.90 |
| ATOM | 4809 | O1  | HOH | W | 24 | 51.995 | 13.231  | 62.486 | 1.00 | 21.98 |
| ATOM | 4810 | O1  | HOH | W | 25 | -2.328 | 13.484  | 27.320 | 1.00 | 20.24 |
| ATOM | 4811 | O1  | HOH | W | 26 | 41.283 | 24.669  | 80.924 | 1.00 | 23.47 |
| ATOM | 4812 | O1  | HOH | W | 27 | 13.869 | -0.367  | 45.406 | 1.00 | 23.14 |
| ATOM | 4813 | O1  | HOH | W | 28 | 15.304 | -9.348  | 27.802 | 1.00 | 21.59 |
| ATOM | 4814 | O1  | HOH | W | 29 | 12.631 | -10.292 | 28.093 | 1.00 | 20.50 |
| ATOM | 4815 | O1  | HOH | W | 30 | 44.431 | 39.247  | 81.240 | 1.00 | 25.13 |
| ATOM | 4816 | O1  | HOH | W | 31 | -0.865 | -4.102  | 45.807 | 1.00 | 17.03 |
| ATOM | 4817 | O1  | HOH | W | 32 | 56.944 | 30.639  | 57.225 | 1.00 | 27.48 |
| ATOM | 4818 | O1  | HOH | W | 33 | 44.974 | 29.800  | 84.482 | 1.00 | 24.66 |
| ATOM | 4819 | O1  | HOH | W | 34 | 40.344 | 25.679  | 78.385 | 1.00 | 25.40 |
| ATOM | 4820 | O1  | HOH | W | 35 | -0.817 | 11.896  | 36.268 | 1.00 | 27.05 |
| ATOM | 4821 | O1  | HOH | W | 36 | 45.813 | 26.347  | 88.982 | 1.00 | 29.74 |
| ATOM | 4822 | O1  | HOH | W | 37 | 61.459 | 21.495  | 62.950 | 1.00 | 24.86 |
| ATOM | 4823 | O1  | HOH | W | 38 | 61.161 | 30.493  | 78.889 | 1.00 | 24.20 |
| ATOM | 4824 | O1  | HOH | W | 39 | 18.380 | -0.097  | 25.182 | 1.00 | 20.65 |
| ATOM | 4825 | O1  | HOH | W | 40 | 51.721 | 30.553  | 83.500 | 1.00 | 23.95 |
| ATOM | 4826 | O1  | HOH | W | 41 | 44.911 | 34.060  | 54.571 | 1.00 | 25.17 |
| ATOM | 4827 | O1  | HOH | W | 42 | 55.088 | 28.823  | 80.613 | 1.00 | 20.78 |
| ATOM | 4828 | O1  | HOH | W | 43 | 38.439 | 25.424  | 57.676 | 1.00 | 24.32 |
| ATOM | 4829 | O1  | HOH | W | 44 | 17.651 | -4.708  | 24.960 | 1.00 | 23.35 |
| ATOM | 4830 | O1  | HOH | W | 45 | 60.668 | 30.480  | 69.410 | 1.00 | 20.33 |
| ATOM | 4831 | O1  | HOH | W | 46 | 10.176 | -14.189 | 47.531 | 1.00 | 30.12 |
| ATOM | 4832 | O1  | HOH | W | 47 | -0.430 | -5.789  | 47.698 | 1.00 | 31.64 |
| ATOM | 4833 | O1  | HOH | W | 48 | 49.454 | 24.259  | 54.551 | 1.00 | 24.40 |
| ATOM | 4834 | O1  | HOH | W | 49 | 8.659  | -4.775  | 50.631 | 1.00 | 26.30 |
| ATOM | 4835 | O1  | HOH | W | 50 | 8.016  | -21.216 | 43.873 | 1.00 | 28.15 |

**FIGURE 195**

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|      |      |    |     |   |     |         |         |        |      |       |
|------|------|----|-----|---|-----|---------|---------|--------|------|-------|
| ATOM | 4836 | O1 | HOH | W | 51  | 41.695  | 31.267  | 59.043 | 1.00 | 30.73 |
| ATOM | 4837 | O1 | HOH | W | 52  | 0.050   | 1.522   | 45.671 | 1.00 | 24.08 |
| ATOM | 4838 | O1 | HOH | W | 53  | 9.328   | 8.423   | 41.215 | 1.00 | 24.60 |
| ATOM | 4839 | O1 | HOH | W | 54  | 18.246  | -7.424  | 47.752 | 1.00 | 27.95 |
| ATOM | 4840 | O1 | HOH | W | 55  | 17.680  | -18.968 | 48.425 | 1.00 | 49.05 |
| ATOM | 4841 | O1 | HOH | W | 56  | 63.663  | 32.033  | 67.334 | 1.00 | 33.07 |
| ATOM | 4842 | O1 | HOH | W | 57  | 12.879  | -8.580  | 21.032 | 1.00 | 30.73 |
| ATOM | 4843 | O1 | HOH | W | 58  | 43.952  | 35.751  | 61.678 | 1.00 | 24.11 |
| ATOM | 4844 | O1 | HOH | W | 59  | 5.457   | 2.609   | 21.937 | 1.00 | 33.95 |
| ATOM | 4845 | O1 | HOH | W | 60  | 41.656  | 34.732  | 60.883 | 1.00 | 26.67 |
| ATOM | 4846 | O1 | HOH | W | 61  | 10.826  | -7.011  | 21.512 | 1.00 | 26.24 |
| ATOM | 4847 | O1 | HOH | W | 62  | 46.866  | 32.271  | 55.142 | 1.00 | 28.91 |
| ATOM | 4848 | O1 | HOH | W | 63  | -4.848  | -11.748 | 39.346 | 1.00 | 22.84 |
| ATOM | 4849 | O1 | HOH | W | 64  | -1.807  | -15.828 | 33.871 | 1.00 | 27.34 |
| ATOM | 4850 | O1 | HOH | W | 65  | 15.309  | -8.364  | 24.800 | 1.00 | 25.02 |
| ATOM | 4851 | O1 | HOH | W | 66  | 10.589  | -3.957  | 17.825 | 1.00 | 26.51 |
| ATOM | 4852 | O1 | HOH | W | 67  | 53.967  | 24.496  | 54.681 | 1.00 | 44.06 |
| ATOM | 4853 | O1 | HOH | W | 68  | 24.990  | -11.936 | 38.629 | 1.00 | 28.80 |
| ATOM | 4854 | O1 | HOH | W | 69  | 7.664   | 0.885   | 20.675 | 1.00 | 28.07 |
| ATOM | 4855 | O1 | HOH | W | 70  | 59.900  | 18.836  | 77.896 | 1.00 | 40.35 |
| ATOM | 4856 | O1 | HOH | W | 71  | 45.172  | 16.962  | 74.854 | 1.00 | 28.34 |
| ATOM | 4857 | O1 | HOH | W | 72  | -7.743  | -7.173  | 31.484 | 1.00 | 26.07 |
| ATOM | 4858 | O1 | HOH | W | 73  | 62.769  | 33.034  | 57.586 | 1.00 | 26.41 |
| ATOM | 4859 | O1 | HOH | W | 74  | 1.944   | -14.302 | 44.406 | 1.00 | 26.86 |
| ATOM | 4860 | O1 | HOH | W | 75  | 23.222  | -0.340  | 29.959 | 1.00 | 22.19 |
| ATOM | 4861 | O1 | HOH | W | 76  | -0.197  | -0.646  | 21.222 | 1.00 | 27.09 |
| ATOM | 4862 | O1 | HOH | W | 77  | 42.078  | 33.736  | 57.956 | 1.00 | 26.98 |
| ATOM | 4863 | O1 | HOH | W | 78  | 57.402  | 25.819  | 56.138 | 1.00 | 32.63 |
| ATOM | 4864 | O1 | HOH | W | 79  | 55.439  | 12.986  | 71.228 | 1.00 | 29.87 |
| ATOM | 4865 | O1 | HOH | W | 80  | 34.396  | 8.529   | 61.576 | 1.00 | 43.51 |
| ATOM | 4866 | O1 | HOH | W | 81  | 47.286  | 29.177  | 51.681 | 1.00 | 31.35 |
| ATOM | 4867 | O1 | HOH | W | 82  | 30.677  | 31.060  | 77.998 | 1.00 | 47.26 |
| ATOM | 4868 | O1 | HOH | W | 83  | 41.588  | 15.444  | 81.328 | 1.00 | 41.21 |
| ATOM | 4869 | O1 | HOH | W | 84  | 2.486   | 5.248   | 46.367 | 1.00 | 34.85 |
| ATOM | 4870 | O1 | HOH | W | 85  | 63.709  | 21.021  | 72.928 | 1.00 | 28.76 |
| ATOM | 4871 | O1 | HOH | W | 86  | 27.619  | 8.328   | 44.050 | 1.00 | 31.73 |
| ATOM | 4872 | O1 | HOH | W | 87  | -5.332  | -10.734 | 36.523 | 1.00 | 25.53 |
| ATOM | 4873 | O1 | HOH | W | 88  | 62.256  | 24.240  | 57.795 | 1.00 | 27.98 |
| ATOM | 4874 | O1 | HOH | W | 89  | 7.339   | -1.362  | 55.174 | 1.00 | 27.75 |
| ATOM | 4875 | O1 | HOH | W | 90  | -3.541  | -2.818  | 46.374 | 1.00 | 29.31 |
| ATOM | 4876 | O1 | HOH | W | 91  | 12.753  | 0.559   | 47.705 | 1.00 | 25.52 |
| ATOM | 4877 | O1 | HOH | W | 92  | 52.949  | 39.174  | 79.040 | 1.00 | 31.30 |
| ATOM | 4878 | O1 | HOH | W | 93  | 36.070  | 32.961  | 80.601 | 1.00 | 30.93 |
| ATOM | 4879 | O1 | HOH | W | 94  | 59.810  | 36.762  | 74.769 | 1.00 | 30.79 |
| ATOM | 4880 | O1 | HOH | W | 95  | -12.875 | 5.864   | 27.849 | 1.00 | 26.59 |
| ATOM | 4881 | O1 | HOH | W | 96  | 53.121  | 29.855  | 85.728 | 1.00 | 31.07 |
| ATOM | 4882 | O1 | HOH | W | 97  | 51.540  | 25.787  | 52.492 | 1.00 | 31.52 |
| ATOM | 4883 | O1 | HOH | W | 98  | 18.594  | -19.849 | 45.929 | 1.00 | 43.83 |
| ATOM | 4884 | O1 | HOH | W | 99  | -1.532  | -18.000 | 43.060 | 1.00 | 30.93 |
| ATOM | 4885 | O1 | HOH | W | 100 | 42.535  | 36.857  | 53.627 | 1.00 | 38.22 |
| ATOM | 4886 | O1 | HOH | W | 101 | 56.933  | 34.861  | 60.367 | 1.00 | 32.82 |
| ATOM | 4887 | O1 | HOH | W | 102 | 25.851  | -1.470  | 29.859 | 1.00 | 36.64 |

**FIGURE 196**



|      |      |    |           |         |         |        |      |       |
|------|------|----|-----------|---------|---------|--------|------|-------|
| ATOM | 4888 | O1 | HOH W 103 | 0.077   | -10.003 | 25.584 | 1.00 | 32.46 |
| ATOM | 4889 | O1 | HOH W 104 | 6.037   | -0.243  | 18.292 | 1.00 | 42.47 |
| ATOM | 4890 | O1 | HOH W 105 | -5.627  | -8.277  | 21.845 | 1.00 | 34.15 |
| ATOM | 4891 | O1 | HOH W 106 | 4.857   | 13.360  | 30.883 | 1.00 | 31.69 |
| ATOM | 4892 | O1 | HOH W 107 | 5.308   | 15.537  | 21.988 | 1.00 | 25.42 |
| ATOM | 4893 | O1 | HOH W 108 | 6.752   | -6.565  | 51.673 | 1.00 | 33.36 |
| ATOM | 4894 | O1 | HOH W 109 | 58.057  | 40.591  | 69.174 | 1.00 | 29.89 |
| ATOM | 4895 | O1 | HOH W 110 | 58.754  | 7.470   | 62.072 | 1.00 | 35.42 |
| ATOM | 4896 | O1 | HOH W 111 | 3.972   | 1.588   | 20.509 | 1.00 | 37.26 |
| ATOM | 4897 | O1 | HOH W 112 | 53.197  | 17.249  | 55.411 | 1.00 | 35.13 |
| ATOM | 4898 | O1 | HOH W 113 | 36.243  | 21.471  | 51.543 | 1.00 | 48.69 |
| ATOM | 4899 | O1 | HOH W 114 | -0.096  | -4.011  | 20.309 | 1.00 | 39.42 |
| ATOM | 4900 | O1 | HOH W 115 | 49.696  | 32.306  | 84.528 | 1.00 | 35.44 |
| ATOM | 4901 | O1 | HOH W 116 | 16.010  | -16.452 | 31.337 | 1.00 | 44.52 |
| ATOM | 4902 | O1 | HOH W 117 | 54.391  | 30.745  | 82.842 | 1.00 | 30.52 |
| ATOM | 4903 | O1 | HOH W 118 | 69.018  | 18.815  | 64.039 | 1.00 | 33.34 |
| ATOM | 4904 | O1 | HOH W 119 | 39.522  | 30.110  | 57.759 | 1.00 | 23.80 |
| ATOM | 4905 | O1 | HOH W 120 | -10.594 | 2.764   | 34.249 | 1.00 | 29.91 |
| ATOM | 4906 | O1 | HOH W 121 | 3.787   | -7.512  | 50.278 | 1.00 | 24.62 |
| ATOM | 4907 | O1 | HOH W 122 | 53.957  | 23.288  | 80.378 | 1.00 | 30.02 |
| ATOM | 4908 | O1 | HOH W 123 | 18.987  | -16.652 | 40.990 | 1.00 | 30.01 |
| ATOM | 4909 | O1 | HOH W 124 | 3.080   | 7.934   | 45.807 | 1.00 | 36.85 |
| ATOM | 4910 | O1 | HOH W 125 | 55.436  | 7.031   | 65.054 | 1.00 | 41.50 |
| ATOM | 4911 | O1 | HOH W 126 | 12.352  | 9.382   | 48.476 | 1.00 | 33.99 |
| ATOM | 4912 | O1 | HOH W 127 | 14.471  | 6.265   | 26.018 | 1.00 | 42.81 |
| ATOM | 4913 | O1 | HOH W 128 | 43.330  | 38.653  | 51.761 | 1.00 | 46.93 |
| ATOM | 4914 | O1 | HOH W 129 | -5.913  | -20.550 | 38.143 | 1.00 | 33.89 |
| ATOM | 4915 | O1 | HOH W 130 | 20.250  | 3.300   | 47.738 | 1.00 | 34.00 |
| ATOM | 4916 | O1 | HOH W 131 | 7.970   | -2.668  | 16.219 | 1.00 | 35.55 |
| ATOM | 4917 | O1 | HOH W 132 | 61.696  | 45.509  | 74.227 | 1.00 | 35.13 |
| ATOM | 4918 | O1 | HOH W 133 | 53.846  | 13.143  | 73.631 | 1.00 | 39.37 |
| ATOM | 4919 | O1 | HOH W 134 | 29.945  | 17.996  | 36.926 | 1.00 | 46.09 |
| ATOM | 4920 | O1 | HOH W 135 | 58.559  | 11.600  | 62.402 | 1.00 | 26.91 |
| ATOM | 4921 | O1 | HOH W 136 | -7.418  | -5.438  | 40.009 | 1.00 | 30.49 |
| ATOM | 4922 | O1 | HOH W 137 | 40.559  | 41.165  | 64.176 | 1.00 | 45.19 |
| ATOM | 4923 | O1 | HOH W 138 | 49.766  | 27.636  | 50.150 | 1.00 | 29.35 |
| ATOM | 4924 | O1 | HOH W 139 | 65.075  | 22.379  | 57.198 | 1.00 | 35.09 |
| ATOM | 4925 | O1 | HOH W 140 | -8.508  | 3.715   | 36.930 | 1.00 | 34.08 |
| ATOM | 4926 | O1 | HOH W 141 | 58.237  | 33.281  | 56.920 | 1.00 | 33.91 |
| ATOM | 4927 | O1 | HOH W 142 | 59.723  | 42.167  | 67.906 | 1.00 | 31.58 |
| ATOM | 4928 | O1 | HOH W 143 | 62.056  | 30.740  | 54.701 | 1.00 | 46.78 |
| ATOM | 4929 | O1 | HOH W 144 | 1.919   | 3.683   | 26.777 | 1.00 | 58.65 |
| ATOM | 4930 | O1 | HOH W 145 | 0.229   | 8.607   | 19.127 | 1.00 | 28.35 |
| ATOM | 4931 | O1 | HOH W 146 | 12.101  | 11.343  | 20.627 | 1.00 | 49.67 |
| ATOM | 4932 | O1 | HOH W 147 | 23.889  | -5.655  | 45.864 | 1.00 | 40.68 |
| ATOM | 4933 | O1 | HOH W 148 | 41.109  | 26.972  | 47.802 | 1.00 | 38.59 |
| ATOM | 4934 | O1 | HOH W 149 | 61.067  | 15.824  | 56.464 | 1.00 | 36.37 |
| ATOM | 4935 | O1 | HOH W 150 | 53.684  | 36.619  | 56.025 | 1.00 | 38.94 |
| ATOM | 4936 | O1 | HOH W 151 | 9.718   | 4.642   | 49.998 | 1.00 | 29.80 |
| ATOM | 4937 | O1 | HOH W 152 | 15.016  | -11.381 | 20.564 | 1.00 | 35.94 |
| ATOM | 4938 | O1 | HOH W 153 | -8.503  | 6.204   | 36.690 | 1.00 | 33.15 |
| ATOM | 4939 | O1 | HOH W 154 | 52.945  | 32.067  | 87.165 | 1.00 | 38.96 |

**FIGURE 197**

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|      |      |    |           |         |         |        |      |       |
|------|------|----|-----------|---------|---------|--------|------|-------|
| ATOM | 4940 | O1 | HOH W 155 | -3.303  | -17.298 | 32.155 | 1.00 | 30.64 |
| ATOM | 4941 | O1 | HOH W 156 | 43.328  | 22.392  | 52.292 | 1.00 | 47.87 |
| ATOM | 4942 | O1 | HOH W 157 | 28.970  | 3.140   | 30.250 | 1.00 | 36.23 |
| ATOM | 4943 | O1 | HOH W 158 | 26.533  | -4.056  | 30.628 | 1.00 | 35.32 |
| ATOM | 4944 | O1 | HOH W 159 | 3.437   | 3.324   | 18.731 | 1.00 | 37.41 |
| ATOM | 4945 | O1 | HOH W 160 | 12.257  | 5.668   | 24.272 | 1.00 | 33.12 |
| ATOM | 4946 | O1 | HOH W 161 | 28.150  | 0.298   | 30.479 | 1.00 | 34.00 |
| ATOM | 4947 | O1 | HOH W 162 | -17.348 | -19.031 | 28.122 | 1.00 | 36.82 |
| ATOM | 4948 | O1 | HOH W 163 | -0.825  | -8.283  | 21.905 | 1.00 | 38.81 |
| ATOM | 4949 | O1 | HOH W 164 | 33.831  | 22.123  | 80.266 | 1.00 | 41.38 |
| ATOM | 4950 | O1 | HOH W 165 | 49.420  | 49.137  | 70.663 | 1.00 | 48.62 |
| ATOM | 4951 | O1 | HOH W 166 | 50.346  | 11.884  | 65.231 | 1.00 | 44.32 |
| ATOM | 4952 | O1 | HOH W 167 | 6.773   | 13.068  | 43.904 | 1.00 | 50.36 |
| ATOM | 4953 | O1 | HOH W 168 | 56.962  | 16.533  | 53.665 | 1.00 | 38.99 |
| ATOM | 4954 | O1 | HOH W 169 | 19.408  | 8.728   | 24.340 | 1.00 | 35.51 |
| ATOM | 4955 | O1 | HOH W 170 | -5.185  | 6.989   | 42.383 | 1.00 | 48.15 |
| ATOM | 4956 | O1 | HOH W 171 | 33.871  | 8.380   | 22.002 | 1.00 | 42.56 |
| ATOM | 4957 | O1 | HOH W 172 | 32.356  | 27.890  | 84.104 | 1.00 | 38.54 |
| ATOM | 4958 | O1 | HOH W 173 | -1.961  | 0.606   | 20.306 | 1.00 | 37.03 |
| ATOM | 4959 | O1 | HOH W 174 | 62.208  | 29.832  | 76.581 | 1.00 | 55.22 |
| ATOM | 4960 | O1 | HOH W 175 | 33.040  | 26.033  | 62.143 | 1.00 | 33.40 |
| ATOM | 4961 | O1 | HOH W 176 | 17.532  | -14.378 | 31.456 | 1.00 | 33.99 |
| ATOM | 4962 | O1 | HOH W 177 | 37.206  | 7.422   | 74.312 | 1.00 | 38.76 |
| ATOM | 4963 | O1 | HOH W 178 | 29.817  | 29.620  | 62.244 | 1.00 | 43.78 |
| ATOM | 4964 | O1 | HOH W 179 | 2.238   | -5.806  | 48.797 | 1.00 | 24.11 |
| ATOM | 4965 | O1 | HOH W 180 | 50.166  | 25.503  | 48.673 | 1.00 | 31.60 |
| ATOM | 4966 | O1 | HOH W 181 | 58.506  | 42.575  | 64.866 | 1.00 | 35.82 |
| ATOM | 4967 | O1 | HOH W 182 | 66.265  | 21.921  | 70.420 | 1.00 | 39.64 |
| ATOM | 4968 | O1 | HOH W 183 | 0.671   | -9.941  | 18.215 | 1.00 | 52.37 |
| ATOM | 4969 | O1 | HOH W 184 | 5.293   | 12.702  | 45.868 | 1.00 | 64.96 |
| ATOM | 4970 | O1 | HOH W 185 | 26.178  | 16.910  | 42.036 | 1.00 | 39.26 |
| ATOM | 4971 | O1 | HOH W 186 | 1.316   | -1.635  | 54.945 | 1.00 | 32.69 |
| ATOM | 4972 | O1 | HOH W 187 | 15.079  | 11.723  | 21.275 | 1.00 | 48.90 |
| ATOM | 4973 | O1 | HOH W 188 | 58.780  | 8.778   | 52.598 | 1.00 | 55.31 |
| ATOM | 4974 | O1 | HOH W 189 | -1.566  | -17.744 | 29.231 | 1.00 | 40.69 |
| ATOM | 4975 | O1 | HOH W 190 | -1.443  | -20.552 | 29.054 | 1.00 | 36.00 |
| ATOM | 4976 | O1 | HOH W 191 | 40.753  | 36.433  | 75.429 | 1.00 | 40.90 |
| ATOM | 4977 | O1 | HOH W 192 | 43.705  | 20.194  | 83.394 | 1.00 | 38.59 |
| ATOM | 4978 | O1 | HOH W 193 | 13.952  | 8.216   | 50.830 | 1.00 | 55.41 |
| ATOM | 4979 | O1 | HOH W 194 | 17.477  | -1.718  | 14.946 | 1.00 | 30.24 |
| ATOM | 4980 | O1 | HOH W 195 | 32.069  | 3.048   | 36.009 | 1.00 | 37.45 |
| ATOM | 4981 | O1 | HOH W 196 | 49.867  | 21.149  | 90.949 | 1.00 | 40.22 |
| ATOM | 4982 | O1 | HOH W 197 | 31.011  | 39.913  | 82.015 | 1.00 | 44.40 |
| ATOM | 4983 | O1 | HOH W 198 | 3.768   | 7.854   | 20.763 | 1.00 | 37.31 |
| ATOM | 4984 | O1 | HOH W 199 | 36.080  | 45.674  | 78.448 | 1.00 | 51.48 |
| ATOM | 4985 | O1 | HOH W 200 | 41.126  | 8.733   | 35.756 | 1.00 | 45.43 |
| ATOM | 4986 | O1 | HOH W 201 | -3.605  | 9.194   | 21.065 | 1.00 | 42.26 |
| ATOM | 4987 | O1 | HOH W 202 | 45.411  | 20.667  | 52.071 | 1.00 | 47.75 |
| ATOM | 4988 | O1 | HOH W 203 | 22.572  | -2.433  | 51.460 | 1.00 | 51.25 |
| ATOM | 4989 | O1 | HOH W 204 | -2.340  | 18.437  | 23.217 | 1.00 | 35.94 |
| ATOM | 4990 | O1 | HOH W 205 | 4.213   | 5.779   | 19.058 | 1.00 | 42.01 |
| ATOM | 4991 | O1 | HOH W 206 | -0.746  | 1.998   | 51.309 | 1.00 | 32.75 |

**FIGURE 198**

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|      |      |    |     |   |     |         |         |        |      |       |
|------|------|----|-----|---|-----|---------|---------|--------|------|-------|
| ATOM | 4992 | O1 | HOH | W | 207 | 28.139  | 33.211  | 71.066 | 1.00 | 52.64 |
| ATOM | 4993 | O1 | HOH | W | 208 | 45.744  | 7.612   | 66.653 | 1.00 | 41.29 |
| ATOM | 4994 | O1 | HOH | W | 209 | 36.066  | 48.240  | 71.868 | 1.00 | 37.65 |
| ATOM | 4995 | O1 | HOH | W | 210 | 27.068  | 31.927  | 66.243 | 1.00 | 45.28 |
| ATOM | 4996 | O1 | HOH | W | 211 | 6.224   | 6.872   | 49.187 | 1.00 | 28.10 |
| ATOM | 4997 | O1 | HOH | W | 212 | -4.674  | 3.941   | 19.505 | 1.00 | 49.63 |
| ATOM | 4998 | O1 | HOH | W | 213 | 36.180  | 26.038  | 50.897 | 1.00 | 39.62 |
| ATOM | 4999 | O1 | HOH | W | 214 | 43.768  | 26.501  | 91.776 | 1.00 | 47.54 |
| ATOM | 5000 | O1 | HOH | W | 215 | 23.227  | -12.725 | 42.616 | 1.00 | 47.18 |
| ATOM | 5001 | O1 | HOH | W | 216 | -5.818  | -21.605 | 40.616 | 1.00 | 37.05 |
| ATOM | 5002 | O1 | HOH | W | 217 | 31.418  | -0.721  | 30.887 | 1.00 | 50.68 |
| ATOM | 5003 | O1 | HOH | W | 218 | 30.636  | 27.485  | 62.006 | 1.00 | 46.74 |
| ATOM | 5004 | O1 | HOH | W | 219 | 26.116  | 18.310  | 75.358 | 1.00 | 48.38 |
| ATOM | 5005 | O1 | HOH | W | 220 | 1.345   | -9.074  | 48.599 | 1.00 | 38.50 |
| ATOM | 5006 | O1 | HOH | W | 221 | 0.416   | -1.086  | 17.311 | 1.00 | 48.92 |
| ATOM | 5007 | O1 | HOH | W | 222 | 54.434  | 21.262  | 61.419 | 1.00 | 42.93 |
| ATOM | 5008 | O1 | HOH | W | 223 | 51.386  | 9.817   | 55.916 | 1.00 | 33.89 |
| ATOM | 5009 | O1 | HOH | W | 224 | 47.376  | 31.902  | 85.186 | 1.00 | 47.01 |
| ATOM | 5010 | O1 | HOH | W | 225 | 14.573  | 9.677   | 49.224 | 1.00 | 33.72 |
| ATOM | 5011 | O1 | HOH | W | 226 | 53.818  | 34.420  | 83.299 | 1.00 | 40.34 |
| ATOM | 5012 | O1 | HOH | W | 227 | 11.775  | 4.191   | 51.814 | 1.00 | 46.81 |
| ATOM | 5013 | O1 | HOH | W | 228 | 36.320  | 19.863  | 21.440 | 1.00 | 41.37 |
| ATOM | 5014 | O1 | HOH | W | 229 | 15.790  | 10.248  | 47.362 | 1.00 | 37.82 |
| ATOM | 5015 | O1 | HOH | W | 230 | 1.272   | 11.705  | 38.927 | 1.00 | 32.13 |
| ATOM | 5016 | O1 | HOH | W | 231 | -7.721  | 2.573   | 21.097 | 1.00 | 38.10 |
| ATOM | 5017 | O1 | HOH | W | 232 | 53.283  | 19.471  | 53.553 | 1.00 | 38.71 |
| ATOM | 5018 | O1 | HOH | W | 233 | 51.950  | 32.548  | 55.051 | 1.00 | 30.33 |
| ATOM | 5019 | O1 | HOH | W | 234 | 58.877  | 41.394  | 62.179 | 1.00 | 45.27 |
| ATOM | 5020 | O1 | HOH | W | 235 | -8.538  | -1.081  | 21.839 | 1.00 | 39.11 |
| ATOM | 5021 | O1 | HOH | W | 236 | -0.733  | 4.812   | 51.216 | 1.00 | 41.83 |
| ATOM | 5022 | O1 | HOH | W | 237 | 60.623  | 35.681  | 72.217 | 1.00 | 39.90 |
| ATOM | 5023 | O1 | HOH | W | 238 | 57.744  | 28.339  | 55.220 | 1.00 | 37.07 |
| ATOM | 5024 | O1 | HOH | W | 239 | 59.092  | 12.614  | 50.910 | 1.00 | 48.79 |
| ATOM | 5025 | O1 | HOH | W | 240 | 68.091  | 31.724  | 68.601 | 1.00 | 34.66 |
| ATOM | 5026 | O1 | HOH | W | 241 | 63.691  | 18.438  | 72.638 | 1.00 | 33.62 |
| ATOM | 5027 | O1 | HOH | W | 242 | 53.127  | 41.929  | 58.612 | 1.00 | 47.21 |
| ATOM | 5028 | O1 | HOH | W | 243 | 1.457   | -17.227 | 23.707 | 1.00 | 48.59 |
| ATOM | 5029 | O1 | HOH | W | 244 | 44.599  | 4.374   | 53.989 | 1.00 | 55.66 |
| ATOM | 5030 | O1 | HOH | W | 245 | -2.827  | 19.837  | 25.584 | 1.00 | 44.10 |
| ATOM | 5031 | O1 | HOH | W | 246 | 22.401  | -9.408  | 51.289 | 1.00 | 46.21 |
| ATOM | 5032 | O1 | HOH | W | 247 | -7.242  | -11.447 | 30.436 | 1.00 | 45.75 |
| ATOM | 5033 | O1 | HOH | W | 248 | 35.419  | 11.112  | 74.634 | 1.00 | 40.36 |
| ATOM | 5034 | O1 | HOH | W | 249 | 49.132  | 5.615   | 57.803 | 1.00 | 41.51 |
| ATOM | 5035 | O1 | HOH | W | 250 | -12.594 | 4.646   | 35.004 | 1.00 | 44.27 |
| ATOM | 5036 | O1 | HOH | W | 251 | -12.226 | 3.502   | 24.096 | 1.00 | 53.57 |
| ATOM | 5037 | O1 | HOH | W | 252 | 49.280  | 12.394  | 79.591 | 1.00 | 54.74 |
| ATOM | 5038 | O1 | HOH | W | 253 | 44.128  | 17.693  | 48.227 | 1.00 | 50.05 |
| ATOM | 5039 | O1 | HOH | W | 254 | 2.013   | -8.971  | 51.042 | 1.00 | 34.88 |
| ATOM | 5040 | O1 | HOH | W | 255 | 29.402  | -6.675  | 32.345 | 1.00 | 54.78 |
| ATOM | 5041 | O1 | HOH | W | 256 | 43.680  | 17.273  | 82.570 | 1.00 | 36.27 |
| ATOM | 5042 | O1 | HOH | W | 257 | 31.835  | -0.971  | 66.953 | 1.00 | 53.67 |
| ATOM | 5043 | O1 | HOH | W | 258 | 34.738  | 9.985   | 59.599 | 1.00 | 38.24 |

**FIGURE 199**

|      |      |    |           |         |         |        |      |       |
|------|------|----|-----------|---------|---------|--------|------|-------|
| ATOM | 5044 | O1 | HOH W 259 | 52.495  | 11.009  | 53.739 | 1.00 | 47.65 |
| ATOM | 5045 | O1 | HOH W 260 | 0.140   | -7.165  | 52.324 | 1.00 | 48.04 |
| ATOM | 5046 | O1 | HOH W 261 | 64.908  | 25.810  | 56.847 | 1.00 | 47.20 |
| ATOM | 5047 | O1 | HOH W 262 | 54.501  | 32.978  | 55.500 | 1.00 | 42.65 |
| ATOM | 5048 | O1 | HOH W 263 | 38.723  | 39.573  | 64.125 | 1.00 | 44.25 |
| ATOM | 5049 | O1 | HOH W 264 | 60.016  | 5.683   | 60.372 | 1.00 | 39.48 |
| ATOM | 5050 | O1 | HOH W 265 | 41.596  | 40.187  | 50.813 | 1.00 | 39.03 |
| ATOM | 5051 | O1 | HOH W 266 | 9.560   | 17.462  | 32.534 | 1.00 | 35.34 |
| ATOM | 5052 | O1 | HOH W 267 | 3.163   | -20.952 | 48.609 | 1.00 | 33.97 |
| ATOM | 5053 | O1 | HOH W 268 | 16.265  | 18.009  | 17.553 | 1.00 | 51.71 |
| ATOM | 5054 | O1 | HOH W 269 | 22.132  | 26.469  | 35.632 | 1.00 | 49.25 |
| ATOM | 5055 | O1 | HOH W 270 | 0.202   | 17.702  | 30.444 | 1.00 | 39.18 |
| ATOM | 5056 | O1 | HOH W 271 | 28.128  | 10.379  | 42.510 | 1.00 | 41.98 |
| ATOM | 5057 | O1 | HOH W 272 | 19.729  | -16.688 | 38.739 | 1.00 | 29.83 |
| ATOM | 5058 | O1 | HOH W 273 | 37.288  | 16.310  | 56.333 | 1.00 | 54.08 |
| ATOM | 5059 | O1 | HOH W 274 | 26.953  | 23.484  | 61.752 | 1.00 | 50.25 |
| ATOM | 5060 | O1 | HOH W 275 | 44.052  | 42.974  | 56.507 | 1.00 | 45.06 |
| ATOM | 5061 | O1 | HOH W 276 | 25.652  | 3.648   | 70.742 | 1.00 | 42.16 |
| ATOM | 5062 | O1 | HOH W 277 | 1.252   | 3.132   | 54.632 | 1.00 | 46.31 |
| ATOM | 5063 | O1 | HOH W 278 | 52.770  | 49.829  | 63.294 | 1.00 | 42.77 |
| ATOM | 5064 | O1 | HOH W 279 | -2.597  | 8.623   | 42.111 | 1.00 | 42.65 |
| ATOM | 5065 | O1 | HOH W 280 | 2.122   | -5.441  | 52.479 | 1.00 | 50.02 |
| ATOM | 5066 | O1 | HOH W 281 | 51.073  | 19.397  | 80.420 | 1.00 | 48.41 |
| ATOM | 5067 | O1 | HOH W 282 | 22.162  | 16.861  | 29.165 | 1.00 | 44.50 |
| ATOM | 5068 | O1 | HOH W 283 | 11.469  | 25.200  | 29.589 | 1.00 | 50.84 |
| ATOM | 5069 | O1 | HOH W 284 | 23.699  | 3.262   | 46.867 | 1.00 | 46.89 |
| ATOM | 5070 | O1 | HOH W 285 | 45.993  | 9.491   | 73.544 | 1.00 | 47.59 |
| ATOM | 5071 | O1 | HOH W 286 | 34.089  | 35.336  | 54.479 | 1.00 | 49.25 |
| ATOM | 5072 | O1 | HOH W 287 | 27.009  | -10.733 | 37.488 | 1.00 | 33.68 |
| ATOM | 5073 | O1 | HOH W 288 | 52.692  | 21.442  | 83.608 | 1.00 | 42.65 |
| ATOM | 5074 | O1 | HOH W 289 | 31.129  | 22.350  | 28.703 | 1.00 | 42.85 |
| ATOM | 5075 | O1 | HOH W 290 | 36.979  | 25.478  | 48.592 | 1.00 | 35.15 |
| ATOM | 5076 | O1 | HOH W 291 | 59.056  | 24.357  | 55.498 | 1.00 | 42.95 |
| ATOM | 5077 | O1 | HOH W 292 | 45.058  | 19.677  | 57.915 | 1.00 | 35.81 |
| ATOM | 5078 | O1 | HOH W 293 | 27.531  | 31.666  | 63.768 | 1.00 | 55.59 |
| ATOM | 5079 | O1 | HOH W 294 | 15.733  | 8.228   | 20.545 | 1.00 | 55.53 |
| ATOM | 5080 | O1 | HOH W 295 | 21.402  | 1.241   | 51.437 | 1.00 | 51.66 |
| ATOM | 5081 | O1 | HOH W 296 | 24.337  | -2.308  | 23.410 | 1.00 | 40.84 |
| ATOM | 5082 | O1 | HOH W 297 | 45.597  | 49.644  | 86.607 | 1.00 | 60.74 |
| ATOM | 5083 | O1 | HOH W 298 | 48.392  | 7.844   | 54.894 | 1.00 | 40.30 |
| ATOM | 5084 | O1 | HOH W 299 | 10.706  | -0.247  | 53.887 | 1.00 | 36.83 |
| ATOM | 5085 | O1 | HOH W 300 | 30.841  | 6.772   | 42.114 | 1.00 | 46.90 |
| ATOM | 5086 | O1 | HOH W 301 | 56.984  | 31.594  | 84.598 | 1.00 | 64.61 |
| ATOM | 5087 | O1 | HOH W 302 | 23.975  | 0.753   | 21.900 | 1.00 | 58.72 |
| ATOM | 5088 | O1 | HOH W 303 | 25.943  | -3.970  | 26.011 | 1.00 | 34.27 |
| ATOM | 5089 | O1 | HOH W 304 | 57.745  | 27.571  | 81.771 | 1.00 | 39.39 |
| ATOM | 5090 | O1 | HOH W 305 | 8.725   | 13.816  | 46.139 | 1.00 | 62.61 |
| ATOM | 5091 | O1 | HOH W 306 | 9.642   | -2.831  | 53.313 | 1.00 | 48.15 |
| ATOM | 5092 | O1 | HOH W 307 | -12.355 | -6.712  | 32.342 | 1.00 | 40.12 |
| ATOM | 5093 | O1 | HOH W 308 | 10.024  | 7.396   | 49.256 | 1.00 | 37.70 |
| ATOM | 5094 | O1 | HOH W 309 | 41.071  | 3.104   | 32.909 | 1.00 | 61.81 |
| ATOM | 5095 | O1 | HOH W 310 | 60.474  | 28.281  | 80.505 | 1.00 | 58.55 |

**FIGURE 200**

|      |      |    |           |        |         |        |      |       |
|------|------|----|-----------|--------|---------|--------|------|-------|
| ATOM | 5096 | O1 | HOH W 311 | -0.719 | 1.660   | 54.184 | 1.00 | 46.99 |
| ATOM | 5097 | O1 | HOH W 312 | 42.157 | 0.641   | 32.043 | 1.00 | 61.15 |
| ATOM | 5098 | O1 | HOH W 313 | 26.844 | 31.094  | 74.091 | 1.00 | 57.31 |
| ATOM | 5099 | O1 | HOH W 314 | 7.696  | 11.428  | 47.893 | 1.00 | 49.96 |
| ATOM | 5100 | O1 | HOH W 315 | 54.048 | 21.906  | 53.414 | 1.00 | 50.41 |
| ATOM | 5101 | O1 | HOH W 316 | 47.093 | 3.308   | 57.181 | 1.00 | 49.89 |
| ATOM | 5102 | O1 | HOH W 317 | 0.538  | 11.547  | 46.107 | 1.00 | 65.71 |
| ATOM | 5103 | O1 | HOH W 318 | 8.860  | 16.730  | 39.751 | 1.00 | 67.14 |
| ATOM | 5104 | O1 | HOH W 319 | 17.788 | -19.138 | 29.587 | 1.00 | 65.65 |
| ATOM | 5105 | O1 | HOH W 320 | 19.712 | 14.524  | 17.149 | 1.00 | 66.48 |
| ATOM | 5106 | O1 | HOH W 321 | -1.219 | -11.550 | 22.358 | 1.00 | 64.74 |
| ATOM | 5107 | O1 | HOH W 322 | 6.040  | 14.352  | 34.149 | 1.00 | 62.82 |
| ATOM | 5108 | O1 | HOH W 323 | 65.030 | 28.876  | 55.181 | 1.00 | 54.52 |
| ATOM | 5109 | O1 | HOH W 324 | 41.175 | 4.830   | 36.570 | 1.00 | 59.29 |
| ATOM | 5110 | O1 | HOH W 325 | 15.916 | -2.843  | 51.316 | 1.00 | 58.50 |
| ATOM | 5111 | O1 | HOH W 326 | 21.478 | 17.683  | 70.720 | 1.00 | 50.48 |
| END  |      |    |           |        |         |        |      |       |

**FIGURE 201**

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|        |        |        |         |       |       |         |        |                    |
|--------|--------|--------|---------|-------|-------|---------|--------|--------------------|
| CRYST1 | 39.250 | 71.126 | 119.912 | 90.00 | 90.00 | 90.00   |        |                    |
| ATOM   | 1      | N      | LYS     | A     | 19    | -12.134 | 41.491 | 10.114 1.000 47.16 |
| ATOM   | 2      | CA     | LYS     | A     | 19    | -12.088 | 40.464 | 9.085 1.000 46.31  |
| ATOM   | 3      | CB     | LYS     | A     | 19    | -11.200 | 40.822 | 7.902 1.000 46.34  |
| ATOM   | 4      | CG     | LYS     | A     | 19    | -9.707  | 40.790 | 8.149 1.000 42.97  |
| ATOM   | 5      | CD     | LYS     | A     | 19    | -8.945  | 40.965 | 6.847 1.000 43.94  |
| ATOM   | 6      | CE     | LYS     | A     | 19    | -7.609  | 41.670 | 7.059 1.000 39.13  |
| ATOM   | 7      | NZ     | LYS     | A     | 19    | -6.732  | 41.562 | 5.856 1.000 48.25  |
| ATOM   | 8      | C      | LYS     | A     | 19    | -11.602 | 39.144 | 9.702 1.000 47.15  |
| ATOM   | 9      | O      | LYS     | A     | 19    | -10.921 | 39.174 | 10.723 1.000 50.63 |
| ATOM   | 10     | N      | THR     | A     | 20    | -11.999 | 38.090 | 9.024 1.000 38.61  |
| ATOM   | 11     | CA     | THR     | A     | 20    | -11.875 | 36.698 | 9.401 1.000 42.80  |
| ATOM   | 12     | CB     | THR     | A     | 20    | -13.310 | 36.133 | 9.502 1.000 46.49  |
| ATOM   | 13     | OG1    | THR     | A     | 20    | -13.660 | 36.080 | 10.896 1.000 54.76 |
| ATOM   | 14     | CG2    | THR     | A     | 20    | -13.393 | 34.742 | 8.933 1.000 40.58  |
| ATOM   | 15     | C      | THR     | A     | 20    | -11.069 | 35.879 | 8.414 1.000 38.96  |
| ATOM   | 16     | O      | THR     | A     | 20    | -10.606 | 34.774 | 8.695 1.000 26.83  |
| ATOM   | 17     | N      | SER     | A     | 21    | -10.899 | 36.432 | 7.211 1.000 27.43  |
| ATOM   | 18     | CA     | SER     | A     | 21    | -10.213 | 35.731 | 6.137 1.000 21.10  |
| ATOM   | 19     | CB     | SER     | A     | 21    | -11.193 | 34.767 | 5.449 1.000 34.39  |
| ATOM   | 20     | OG     | SER     | A     | 21    | -10.929 | 34.678 | 4.055 1.000 44.20  |
| ATOM   | 21     | C      | SER     | A     | 21    | -9.647  | 36.730 | 5.144 1.000 25.82  |
| ATOM   | 22     | O      | SER     | A     | 21    | -10.151 | 37.858 | 5.158 1.000 39.09  |
| ATOM   | 23     | N      | CYS     | A     | 22    | -8.669  | 36.373 | 4.325 1.000 26.63  |
| ATOM   | 24     | CA     | CYS     | A     | 22    | -8.080  | 37.358 | 3.404 1.000 29.32  |
| ATOM   | 25     | CB     | CYS     | A     | 22    | -7.041  | 38.266 | 4.056 1.000 29.54  |
| ATOM   | 26     | SG     | CYS     | A     | 22    | -6.599  | 39.770 | 3.116 1.000 40.23  |
| ATOM   | 27     | C      | CYS     | A     | 22    | -7.445  | 36.575 | 2.264 1.000 28.58  |
| ATOM   | 28     | O      | CYS     | A     | 22    | -6.219  | 36.546 | 2.161 1.000 36.15  |
| ATOM   | 29     | N      | PRO     | A     | 23    | -8.315  | 35.942 | 1.482 1.000 31.23  |
| ATOM   | 30     | CA     | PRO     | A     | 23    | -7.853  | 35.032 | 0.450 1.000 28.72  |
| ATOM   | 31     | CB     | PRO     | A     | 23    | -9.120  | 34.324 | -0.025 1.000 32.50 |
| ATOM   | 32     | CG     | PRO     | A     | 23    | -10.228 | 35.253 | 0.317 1.000 32.13  |
| ATOM   | 33     | CD     | PRO     | A     | 23    | -9.784  | 36.062 | 1.490 1.000 33.79  |
| ATOM   | 34     | C      | PRO     | A     | 23    | -7.229  | 35.869 | -0.664 1.000 27.64 |
| ATOM   | 35     | O      | PRO     | A     | 23    | -7.703  | 36.980 | -0.890 1.000 28.84 |
| ATOM   | 36     | N      | ILE     | A     | 24    | -6.205  | 35.309 | -1.275 1.000 25.07 |
| ATOM   | 37     | CA     | ILE     | A     | 24    | -5.480  | 35.988 | -2.347 1.000 26.87 |
| ATOM   | 38     | CB     | ILE     | A     | 24    | -4.118  | 36.521 | -1.880 1.000 23.03 |
| ATOM   | 39     | CG1    | ILE     | A     | 24    | -4.194  | 37.387 | -0.616 1.000 32.69 |
| ATOM   | 40     | CD1    | ILE     | A     | 24    | -4.803  | 38.749 | -0.870 1.000 36.67 |
| ATOM   | 41     | CG2    | ILE     | A     | 24    | -3.411  | 37.301 | -2.982 1.000 35.11 |
| ATOM   | 42     | C      | ILE     | A     | 24    | -5.297  | 35.003 | -3.489 1.000 23.25 |
| ATOM   | 43     | O      | ILE     | A     | 24    | -4.816  | 33.891 | -3.288 1.000 28.71 |
| ATOM   | 44     | N      | LYS     | A     | 25    | -5.703  | 35.414 | -4.692 1.000 28.16 |
| ATOM   | 45     | CA     | LYS     | A     | 25    | -5.530  | 34.603 | -5.877 1.000 28.40 |
| ATOM   | 46     | CB     | LYS     | A     | 25    | -6.067  | 35.296 | -7.130 1.000 34.65 |
| ATOM   | 47     | CG     | LYS     | A     | 25    | -7.546  | 35.653 | -7.058 1.000 38.17 |
| ATOM   | 48     | CD     | LYS     | A     | 25    | -7.944  | 36.538 | -8.227 1.000 48.55 |
| ATOM   | 49     | CE     | LYS     | A     | 25    | -9.420  | 36.915 | -8.158 1.000 55.62 |
| ATOM   | 50     | NZ     | LYS     | A     | 25    | -9.640  | 38.251 | -7.532 1.000 59.24 |
| ATOM   | 51     | C      | LYS     | A     | 25    | -4.034  | 34.363 | -6.051 1.000 26.23 |

**FIGURE 202**

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|      |     |     |     |   |    |        |        |         |       |        |
|------|-----|-----|-----|---|----|--------|--------|---------|-------|--------|
| ATOM | 52  | O   | LYS | A | 25 | -3.283 | 35.312 | -5.797  | 1.000 | 35.63  |
| ATOM | 53  | N   | ILE | A | 26 | -3.655 | 33.153 | -6.449  | 1.000 | 26.51  |
| ATOM | 54  | CA  | ILE | A | 26 | -2.202 | 32.943 | -6.476  | 1.000 | 39.40  |
| ATOM | 55  | CB  | ILE | A | 26 | -1.848 | 31.483 | -6.769  | 1.000 | 41.92  |
| ATOM | 56  | CG1 | ILE | A | 26 | -2.538 | 30.872 | -7.986  | 1.000 | 55.69  |
| ATOM | 57  | CD1 | ILE | A | 26 | -1.953 | 29.527 | -8.398  | 1.000 | 43.15  |
| ATOM | 58  | CG2 | ILE | A | 26 | -2.092 | 30.645 | -5.505  | 1.000 | 30.44  |
| ATOM | 59  | C   | ILE | A | 26 | -1.545 | 33.891 | -7.468  | 1.000 | 49.89  |
| ATOM | 60  | O   | ILE | A | 26 | -0.403 | 34.315 | -7.258  | 1.000 | 61.92  |
| ATOM | 61  | N   | ASN | A | 27 | -2.257 | 34.261 | -8.535  | 1.000 | 47.63  |
| ATOM | 62  | CA  | ASN | A | 27 | -1.622 | 35.182 | -9.489  | 1.000 | 48.85  |
| ATOM | 63  | CB  | ASN | A | 27 | -2.409 | 35.259 | -10.789 | 1.000 | 58.29  |
| ATOM | 64  | CG  | ASN | A | 27 | -3.867 | 35.634 | -10.702 | 1.000 | 64.78  |
| ATOM | 65  | OD1 | ASN | A | 27 | -4.735 | 34.952 | -11.257 | 1.000 | 66.47  |
| ATOM | 66  | ND2 | ASN | A | 27 | -4.181 | 36.732 | -10.026 | 1.000 | 76.39  |
| ATOM | 67  | C   | ASN | A | 27 | -1.419 | 36.560 | -8.875  | 1.000 | 42.84  |
| ATOM | 68  | O   | ASN | A | 27 | -0.555 | 37.314 | -9.323  | 1.000 | 45.62  |
| ATOM | 69  | N   | GLN | A | 28 | -2.197 | 36.926 | -7.856  | 1.000 | 38.86  |
| ATOM | 70  | CA  | GLN | A | 28 | -1.986 | 38.188 | -7.174  | 1.000 | 39.38  |
| ATOM | 71  | CB  | GLN | A | 28 | -3.330 | 38.731 | -6.666  | 1.000 | 44.68  |
| ATOM | 72  | CG  | GLN | A | 28 | -3.622 | 40.150 | -7.123  | 1.000 | 69.70  |
| ATOM | 73  | CD  | GLN | A | 28 | -3.103 | 40.420 | -8.526  | 1.000 | 86.93  |
| ATOM | 74  | OE1 | GLN | A | 28 | -3.225 | 39.566 | -9.412  | 1.000 | 117.05 |
| ATOM | 75  | NE2 | GLN | A | 28 | -2.527 | 41.600 | -8.735  | 1.000 | 74.84  |
| ATOM | 76  | C   | GLN | A | 28 | -1.024 | 38.107 | -5.992  | 1.000 | 38.67  |
| ATOM | 77  | O   | GLN | A | 28 | -0.763 | 39.173 | -5.416  | 1.000 | 27.96  |
| ATOM | 78  | N   | PHE | A | 29 | -0.525 | 36.933 | -5.609  | 1.000 | 36.04  |
| ATOM | 79  | CA  | PHE | A | 29 | 0.171  | 36.807 | -4.326  | 1.000 | 34.34  |
| ATOM | 80  | CB  | PHE | A | 29 | 0.531  | 35.339 | -3.998  | 1.000 | 30.22  |
| ATOM | 81  | CG  | PHE | A | 29 | 0.922  | 35.274 | -2.520  | 1.000 | 26.86  |
| ATOM | 82  | CD1 | PHE | A | 29 | -0.074 | 35.297 | -1.554  | 1.000 | 29.29  |
| ATOM | 83  | CE1 | PHE | A | 29 | 0.225  | 35.248 | -0.203  | 1.000 | 28.67  |
| ATOM | 84  | CZ  | PHE | A | 29 | 1.560  | 35.208 | 0.168   | 1.000 | 38.22  |
| ATOM | 85  | CE2 | PHE | A | 29 | 2.567  | 35.166 | -0.786  | 1.000 | 38.42  |
| ATOM | 86  | CD2 | PHE | A | 29 | 2.249  | 35.197 | -2.134  | 1.000 | 32.07  |
| ATOM | 87  | C   | PHE | A | 29 | 1.448  | 37.636 | -4.193  | 1.000 | 33.30  |
| ATOM | 88  | O   | PHE | A | 29 | 1.580  | 38.350 | -3.187  | 1.000 | 34.15  |
| ATOM | 89  | N   | GLU | A | 30 | 2.352  | 37.531 | -5.149  | 1.000 | 41.14  |
| ATOM | 90  | CA  | GLU | A | 30 | 3.603  | 38.271 | -5.221  | 1.000 | 38.75  |
| ATOM | 91  | CB  | GLU | A | 30 | 4.200  | 38.126 | -6.629  | 1.000 | 41.90  |
| ATOM | 92  | CG  | GLU | A | 30 | 5.619  | 38.657 | -6.739  | 1.000 | 50.56  |
| ATOM | 93  | CD  | GLU | A | 30 | 6.619  | 37.768 | -6.022  | 1.000 | 60.13  |
| ATOM | 94  | OE1 | GLU | A | 30 | 6.912  | 36.658 | -6.515  | 1.000 | 51.89  |
| ATOM | 95  | OE2 | GLU | A | 30 | 7.109  | 38.196 | -4.954  | 1.000 | 80.65  |
| ATOM | 96  | C   | GLU | A | 30 | 3.456  | 39.755 | -4.931  | 1.000 | 38.26  |
| ATOM | 97  | O   | GLU | A | 30 | 4.217  | 40.361 | -4.169  | 1.000 | 39.06  |
| ATOM | 98  | N   | GLY | A | 31 | 2.463  | 40.378 | -5.572  | 1.000 | 33.74  |
| ATOM | 99  | CA  | GLY | A | 31 | 2.321  | 41.815 | -5.409  | 1.000 | 29.48  |
| ATOM | 100 | C   | GLY | A | 31 | 1.552  | 42.106 | -4.143  | 1.000 | 35.24  |
| ATOM | 101 | O   | GLY | A | 31 | 1.757  | 43.141 | -3.521  | 1.000 | 37.25  |
| ATOM | 102 | N   | HIS | A | 32 | 0.678  | 41.149 | -3.786  | 1.000 | 36.89  |
| ATOM | 103 | CA  | HIS | A | 32 | 0.025  | 41.293 | -2.488  | 1.000 | 33.45  |

**FIGURE 203**

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 104 | CB  | HIS | A | 32 | -0.863 | 40.102 | -2.149 | 1.000 | 30.08 |
| ATOM | 105 | CG  | HIS | A | 32 | -1.356 | 40.057 | -0.738 | 1.000 | 25.45 |
| ATOM | 106 | ND1 | HIS | A | 32 | -2.309 | 40.907 | -0.234 | 1.000 | 36.70 |
| ATOM | 107 | CE1 | HIS | A | 32 | -2.555 | 40.630 | 1.038  | 1.000 | 39.89 |
| ATOM | 108 | NE2 | HIS | A | 32 | -1.786 | 39.603 | 1.379  | 1.000 | 36.80 |
| ATOM | 109 | CD2 | HIS | A | 32 | -1.032 | 39.232 | 0.292  | 1.000 | 26.97 |
| ATOM | 110 | C   | HIS | A | 32 | 1.101  | 41.431 | -1.410 | 1.000 | 35.73 |
| ATOM | 111 | O   | HIS | A | 32 | 1.007  | 42.277 | -0.516 | 1.000 | 32.27 |
| ATOM | 112 | N   | PHE | A | 33 | 2.090  | 40.543 | -1.556 | 1.000 | 34.68 |
| ATOM | 113 | CA  | PHE | A | 33 | 3.120  | 40.431 | -0.515 | 1.000 | 32.48 |
| ATOM | 114 | CB  | PHE | A | 33 | 3.828  | 39.071 | -0.591 | 1.000 | 36.84 |
| ATOM | 115 | CG  | PHE | A | 33 | 4.751  | 38.835 | 0.595  | 1.000 | 37.98 |
| ATOM | 116 | CD1 | PHE | A | 33 | 4.471  | 39.433 | 1.812  | 1.000 | 40.95 |
| ATOM | 117 | CE1 | PHE | A | 33 | 5.308  | 39.272 | 2.895  | 1.000 | 43.07 |
| ATOM | 118 | CZ  | PHE | A | 33 | 6.440  | 38.479 | 2.754  | 1.000 | 34.64 |
| ATOM | 119 | CE2 | PHE | A | 33 | 6.724  | 37.866 | 1.554  | 1.000 | 26.60 |
| ATOM | 120 | CD2 | PHE | A | 33 | 5.875  | 38.039 | 0.472  | 1.000 | 32.44 |
| ATOM | 121 | C   | PHE | A | 33 | 4.050  | 41.630 | -0.607 | 1.000 | 36.33 |
| ATOM | 122 | O   | PHE | A | 33 | 4.526  | 42.116 | 0.428  | 1.000 | 41.59 |
| ATOM | 123 | N   | MET | A | 34 | 4.284  | 42.170 | -1.802 | 1.000 | 45.92 |
| ATOM | 124 | CA  | MET | A | 34 | 5.094  | 43.397 | -1.876 | 1.000 | 40.90 |
| ATOM | 125 | CB  | MET | A | 34 | 5.460  | 43.656 | -3.336 | 1.000 | 48.61 |
| ATOM | 126 | CG  | MET | A | 34 | 6.895  | 43.260 | -3.662 | 1.000 | 40.86 |
| ATOM | 127 | SD  | MET | A | 34 | 6.983  | 41.845 | -4.774 | 1.000 | 86.63 |
| ATOM | 128 | CE  | MET | A | 34 | 8.572  | 41.170 | -4.254 | 1.000 | 72.85 |
| ATOM | 129 | C   | MET | A | 34 | 4.383  | 44.588 | -1.259 | 1.000 | 42.23 |
| ATOM | 130 | O   | MET | A | 34 | 4.968  | 45.443 | -0.568 | 1.000 | 50.41 |
| ATOM | 131 | N   | LYS | A | 35 | 3.065  | 44.686 | -1.458 | 1.000 | 34.55 |
| ATOM | 132 | CA  | LYS | A | 35 | 2.351  | 45.788 | -0.795 | 1.000 | 45.08 |
| ATOM | 133 | CB  | LYS | A | 35 | 0.889  | 45.809 | -1.279 | 1.000 | 48.74 |
| ATOM | 134 | CG  | LYS | A | 35 | 0.793  | 46.296 | -2.720 | 1.000 | 51.47 |
| ATOM | 135 | CD  | LYS | A | 35 | -0.509 | 45.889 | -3.382 | 1.000 | 56.83 |
| ATOM | 136 | CE  | LYS | A | 35 | -0.788 | 46.795 | -4.577 | 1.000 | 55.04 |
| ATOM | 137 | NZ  | LYS | A | 35 | -0.993 | 46.020 | -5.830 | 1.000 | 61.49 |
| ATOM | 138 | C   | LYS | A | 35 | 2.417  | 45.703 | 0.717  | 1.000 | 38.13 |
| ATOM | 139 | O   | LYS | A | 35 | 2.575  | 46.713 | 1.419  | 1.000 | 38.53 |
| ATOM | 140 | N   | LEU | A | 36 | 2.293  | 44.483 | 1.267  | 1.000 | 37.05 |
| ATOM | 141 | CA  | LEU | A | 36 | 2.281  | 44.337 | 2.720  | 1.000 | 33.35 |
| ATOM | 142 | CB  | LEU | A | 36 | 1.904  | 42.922 | 3.179  | 1.000 | 29.64 |
| ATOM | 143 | CG  | LEU | A | 36 | 0.453  | 42.474 | 3.024  | 1.000 | 30.10 |
| ATOM | 144 | CD1 | LEU | A | 36 | 0.259  | 41.052 | 3.567  | 1.000 | 35.30 |
| ATOM | 145 | CD2 | LEU | A | 36 | -0.516 | 43.409 | 3.723  | 1.000 | 31.56 |
| ATOM | 146 | C   | LEU | A | 36 | 3.641  | 44.718 | 3.311  | 1.000 | 26.53 |
| ATOM | 147 | O   | LEU | A | 36 | 3.664  | 45.268 | 4.415  | 1.000 | 45.90 |
| ATOM | 148 | N   | GLN | A | 37 | 4.713  | 44.426 | 2.591  | 1.000 | 30.34 |
| ATOM | 149 | CA  | GLN | A | 37 | 6.073  | 44.682 | 3.038  | 1.000 | 46.11 |
| ATOM | 150 | CB  | GLN | A | 37 | 7.038  | 43.727 | 2.321  | 1.000 | 45.16 |
| ATOM | 151 | CG  | GLN | A | 37 | 7.047  | 42.323 | 2.925  | 1.000 | 46.46 |
| ATOM | 152 | CD  | GLN | A | 37 | 7.963  | 41.397 | 2.146  | 1.000 | 41.79 |
| ATOM | 153 | OE1 | GLN | A | 37 | 8.895  | 40.818 | 2.701  | 1.000 | 53.12 |
| ATOM | 154 | NE2 | GLN | A | 37 | 7.682  | 41.253 | 0.854  | 1.000 | 59.23 |
| ATOM | 155 | C   | GLN | A | 37 | 6.554  | 46.116 | 2.816  | 1.000 | 58.12 |

**FIGURE 204**



|      |     |     |     |   |    |        |        |       |       |       |
|------|-----|-----|-----|---|----|--------|--------|-------|-------|-------|
| ATOM | 156 | O   | GLN | A | 37 | 7.585  | 46.535 | 3.366 | 1.000 | 44.71 |
| ATOM | 157 | N   | ALA | A | 38 | 5.820  | 46.878 | 2.014 | 1.000 | 51.00 |
| ATOM | 158 | CA  | ALA | A | 38 | 6.214  | 48.252 | 1.734 | 1.000 | 51.95 |
| ATOM | 159 | CB  | ALA | A | 38 | 5.334  | 48.856 | 0.638 | 1.000 | 33.90 |
| ATOM | 160 | C   | ALA | A | 38 | 6.155  | 49.144 | 2.971 | 1.000 | 53.47 |
| ATOM | 161 | O   | ALA | A | 38 | 5.408  | 48.911 | 3.916 | 1.000 | 39.54 |
| ATOM | 162 | N   | ASP | A | 39 | 6.967  | 50.198 | 2.923 | 1.000 | 54.79 |
| ATOM | 163 | CA  | ASP | A | 39 | 7.037  | 51.192 | 3.990 | 1.000 | 41.76 |
| ATOM | 164 | CB  | ASP | A | 39 | 5.738  | 51.973 | 4.114 | 1.000 | 38.24 |
| ATOM | 165 | CG  | ASP | A | 39 | 5.127  | 52.287 | 2.757 | 1.000 | 53.89 |
| ATOM | 166 | OD1 | ASP | A | 39 | 4.001  | 52.837 | 2.732 | 1.000 | 61.68 |
| ATOM | 167 | OD2 | ASP | A | 39 | 5.750  | 52.000 | 1.707 | 1.000 | 55.37 |
| ATOM | 168 | C   | ASP | A | 39 | 7.401  | 50.477 | 5.289 | 1.000 | 41.78 |
| ATOM | 169 | O   | ASP | A | 39 | 6.886  | 50.753 | 6.369 | 1.000 | 42.20 |
| ATOM | 170 | N   | SER | A | 40 | 8.339  | 49.547 | 5.104 | 1.000 | 41.63 |
| ATOM | 171 | CA  | SER | A | 40 | 8.819  | 48.736 | 6.213 | 1.000 | 39.11 |
| ATOM | 172 | CB  | SER | A | 40 | 9.331  | 49.627 | 7.344 | 1.000 | 45.54 |
| ATOM | 173 | OG  | SER | A | 40 | 10.507 | 50.325 | 6.967 | 1.000 | 63.33 |
| ATOM | 174 | C   | SER | A | 40 | 7.701  | 47.838 | 6.726 | 1.000 | 33.78 |
| ATOM | 175 | O   | SER | A | 40 | 7.500  | 47.791 | 7.939 | 1.000 | 44.33 |
| ATOM | 176 | N   | ASN | A | 41 | 6.979  | 47.158 | 5.831 | 1.000 | 36.63 |
| ATOM | 177 | CA  | ASN | A | 41 | 5.911  | 46.290 | 6.314 | 1.000 | 46.11 |
| ATOM | 178 | CB  | ASN | A | 41 | 6.386  | 45.245 | 7.332 | 1.000 | 39.56 |
| ATOM | 179 | CG  | ASN | A | 41 | 7.336  | 44.240 | 6.734 | 1.000 | 39.34 |
| ATOM | 180 | OD1 | ASN | A | 41 | 7.679  | 43.246 | 7.379 | 1.000 | 66.37 |
| ATOM | 181 | ND2 | ASN | A | 41 | 7.760  | 44.503 | 5.505 | 1.000 | 47.43 |
| ATOM | 182 | C   | ASN | A | 41 | 4.833  | 47.097 | 7.034 | 1.000 | 52.00 |
| ATOM | 183 | O   | ASN | A | 41 | 4.484  | 46.727 | 8.159 | 1.000 | 45.88 |
| ATOM | 184 | N   | TYR | A | 42 | 4.366  | 48.150 | 6.376 | 1.000 | 47.78 |
| ATOM | 185 | CA  | TYR | A | 42 | 3.394  | 49.022 | 7.014 | 1.000 | 48.64 |
| ATOM | 186 | CB  | TYR | A | 42 | 3.181  | 50.305 | 6.197 | 1.000 | 50.57 |
| ATOM | 187 | CG  | TYR | A | 42 | 2.110  | 51.181 | 6.818 | 1.000 | 60.30 |
| ATOM | 188 | CD1 | TYR | A | 42 | 2.315  | 51.798 | 8.049 | 1.000 | 73.71 |
| ATOM | 189 | CE1 | TYR | A | 42 | 1.345  | 52.597 | 8.619 | 1.000 | 79.76 |
| ATOM | 190 | CZ  | TYR | A | 42 | 0.148  | 52.779 | 7.947 | 1.000 | 83.87 |
| ATOM | 191 | OH  | TYR | A | 42 | -0.829 | 53.570 | 8.494 | 1.000 | 96.86 |
| ATOM | 192 | CE2 | TYR | A | 42 | -0.084 | 52.176 | 6.728 | 1.000 | 77.87 |
| ATOM | 193 | CD2 | TYR | A | 42 | 0.899  | 51.382 | 6.173 | 1.000 | 69.62 |
| ATOM | 194 | C   | TYR | A | 42 | 2.080  | 48.272 | 7.202 | 1.000 | 40.91 |
| ATOM | 195 | O   | TYR | A | 42 | 1.518  | 48.233 | 8.297 | 1.000 | 38.94 |
| ATOM | 196 | N   | LEU | A | 43 | 1.628  | 47.688 | 6.094 | 1.000 | 39.86 |
| ATOM | 197 | CA  | LEU | A | 43 | 0.324  | 47.037 | 6.065 | 1.000 | 38.25 |
| ATOM | 198 | CB  | LEU | A | 43 | -0.240 | 46.976 | 4.648 | 1.000 | 34.42 |
| ATOM | 199 | CG  | LEU | A | 43 | -0.625 | 48.329 | 4.021 | 1.000 | 39.05 |
| ATOM | 200 | CD1 | LEU | A | 43 | -0.840 | 48.146 | 2.529 | 1.000 | 35.82 |
| ATOM | 201 | CD2 | LEU | A | 43 | -1.869 | 48.904 | 4.671 | 1.000 | 38.28 |
| ATOM | 202 | C   | LEU | A | 43 | 0.401  | 45.628 | 6.658 | 1.000 | 40.26 |
| ATOM | 203 | O   | LEU | A | 43 | -0.571 | 45.204 | 7.288 | 1.000 | 41.80 |
| ATOM | 204 | N   | LEU | A | 44 | 1.531  | 44.954 | 6.473 | 1.000 | 40.52 |
| ATOM | 205 | CA  | LEU | A | 44 | 1.755  | 43.658 | 7.118 | 1.000 | 40.17 |
| ATOM | 206 | CB  | LEU | A | 44 | 3.181  | 43.148 | 6.903 | 1.000 | 40.11 |
| ATOM | 207 | CG  | LEU | A | 44 | 3.410  | 41.689 | 7.327 | 1.000 | 39.64 |

**FIGURE 205**

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 208 | CD1 | LEU | A | 44 | 4.236  | 40.957 | 6.288  | 1.000 | 46.27 |
| ATOM | 209 | CD2 | LEU | A | 44 | 4.073  | 41.640 | 8.693  | 1.000 | 36.71 |
| ATOM | 210 | C   | LEU | A | 44 | 1.490  | 43.724 | 8.616  | 1.000 | 40.53 |
| ATOM | 211 | O   | LEU | A | 44 | 0.821  | 42.859 | 9.180  | 1.000 | 35.07 |
| ATOM | 212 | N   | SER | A | 45 | 2.019  | 44.759 | 9.269  | 1.000 | 33.52 |
| ATOM | 213 | CA  | SER | A | 45 | 1.856  | 44.909 | 10.710 | 1.000 | 33.03 |
| ATOM | 214 | CB  | SER | A | 45 | 2.871  | 45.946 | 11.228 | 1.000 | 29.94 |
| ATOM | 215 | OG  | SER | A | 45 | 4.137  | 45.710 | 10.612 | 1.000 | 33.78 |
| ATOM | 216 | C   | SER | A | 45 | 0.433  | 45.275 | 11.087 | 1.000 | 36.97 |
| ATOM | 217 | O   | SER | A | 45 | -0.131 | 44.758 | 12.058 | 1.000 | 34.42 |
| ATOM | 218 | N   | LYS | A | 46 | -0.211 | 46.176 | 10.345 | 1.000 | 34.85 |
| ATOM | 219 | CA  | LYS | A | 46 | -1.630 | 46.418 | 10.604 | 1.000 | 31.36 |
| ATOM | 220 | CB  | LYS | A | 46 | -2.199 | 47.461 | 9.636  | 1.000 | 36.80 |
| ATOM | 221 | CG  | LYS | A | 46 | -1.400 | 48.758 | 9.630  | 1.000 | 46.16 |
| ATOM | 222 | CD  | LYS | A | 46 | -2.286 | 49.966 | 9.884  | 1.000 | 50.59 |
| ATOM | 223 | CE  | LYS | A | 46 | -1.915 | 50.631 | 11.197 | 1.000 | 58.31 |
| ATOM | 224 | NZ  | LYS | A | 46 | -0.513 | 51.127 | 11.179 | 1.000 | 66.09 |
| ATOM | 225 | C   | LYS | A | 46 | -2.425 | 45.116 | 10.503 | 1.000 | 31.41 |
| ATOM | 226 | O   | LYS | A | 46 | -3.340 | 44.917 | 11.304 | 1.000 | 42.72 |
| ATOM | 227 | N   | GLU | A | 47 | -2.082 | 44.251 | 9.555  | 1.000 | 27.42 |
| ATOM | 228 | CA  | GLU | A | 47 | -2.810 | 43.006 | 9.332  | 1.000 | 33.85 |
| ATOM | 229 | CB  | GLU | A | 47 | -2.437 | 42.314 | 8.018  | 1.000 | 35.99 |
| ATOM | 230 | CG  | GLU | A | 47 | -3.311 | 41.079 | 7.802  | 1.000 | 36.26 |
| ATOM | 231 | CD  | GLU | A | 47 | -3.301 | 40.603 | 6.369  | 1.000 | 33.51 |
| ATOM | 232 | OE1 | GLU | A | 47 | -4.136 | 41.068 | 5.559  | 1.000 | 34.52 |
| ATOM | 233 | OE2 | GLU | A | 47 | -2.433 | 39.753 | 6.076  | 1.000 | 31.53 |
| ATOM | 234 | C   | GLU | A | 47 | -2.560 | 41.985 | 10.443 | 1.000 | 30.28 |
| ATOM | 235 | O   | GLU | A | 47 | -3.506 | 41.345 | 10.901 | 1.000 | 37.61 |
| ATOM | 236 | N   | TYR | A | 48 | -1.298 | 41.883 | 10.836 | 1.000 | 30.47 |
| ATOM | 237 | CA  | TYR | A | 48 | -0.931 | 41.057 | 11.983 | 1.000 | 29.64 |
| ATOM | 238 | CB  | TYR | A | 48 | 0.590  | 41.107 | 12.208 | 1.000 | 34.11 |
| ATOM | 239 | CG  | TYR | A | 48 | 1.016  | 40.197 | 13.336 | 1.000 | 31.94 |
| ATOM | 240 | CD1 | TYR | A | 48 | 0.866  | 38.821 | 13.183 | 1.000 | 33.96 |
| ATOM | 241 | CE1 | TYR | A | 48 | 1.231  | 37.938 | 14.175 | 1.000 | 32.68 |
| ATOM | 242 | CZ  | TYR | A | 48 | 1.754  | 38.404 | 15.360 | 1.000 | 35.81 |
| ATOM | 243 | OH  | TYR | A | 48 | 2.101  | 37.491 | 16.330 | 1.000 | 39.47 |
| ATOM | 244 | CE2 | TYR | A | 48 | 1.911  | 39.760 | 15.548 | 1.000 | 38.83 |
| ATOM | 245 | CD2 | TYR | A | 48 | 1.542  | 40.648 | 14.540 | 1.000 | 36.26 |
| ATOM | 246 | C   | TYR | A | 48 | -1.712 | 41.530 | 13.202 | 1.000 | 39.70 |
| ATOM | 247 | O   | TYR | A | 48 | -2.201 | 40.748 | 14.015 | 1.000 | 34.67 |
| ATOM | 248 | N   | GLU | A | 49 | -1.839 | 42.852 | 13.334 | 1.000 | 34.55 |
| ATOM | 249 | CA  | GLU | A | 49 | -2.480 | 43.503 | 14.469 | 1.000 | 26.84 |
| ATOM | 250 | CB  | GLU | A | 49 | -2.226 | 45.029 | 14.435 | 1.000 | 31.26 |
| ATOM | 251 | CG  | GLU | A | 49 | -0.796 | 45.295 | 14.919 | 1.000 | 41.28 |
| ATOM | 252 | CD  | GLU | A | 49 | -0.707 | 44.824 | 16.368 | 1.000 | 46.36 |
| ATOM | 253 | OE1 | GLU | A | 49 | 0.167  | 44.004 | 16.694 | 1.000 | 49.76 |
| ATOM | 254 | OE2 | GLU | A | 49 | -1.540 | 45.294 | 17.171 | 1.000 | 64.46 |
| ATOM | 255 | C   | GLU | A | 49 | -3.968 | 43.243 | 14.489 | 1.000 | 17.64 |
| ATOM | 256 | O   | GLU | A | 49 | -4.611 | 43.212 | 15.530 | 1.000 | 31.99 |
| ATOM | 257 | N   | GLU | A | 50 | -4.527 | 43.054 | 13.298 | 1.000 | 24.66 |
| ATOM | 258 | CA  | GLU | A | 50 | -5.942 | 42.729 | 13.220 | 1.000 | 33.35 |
| ATOM | 259 | CB  | GLU | A | 50 | -6.441 | 42.674 | 11.768 | 1.000 | 34.57 |

FIGURE 206

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 260 | CG  | GLU | A | 50 | -6.190  | 43.933 | 10.956 | 1.000 | 42.22 |
| ATOM | 261 | CD  | GLU | A | 50 | -7.128  | 43.945 | 9.750  | 1.000 | 52.34 |
| ATOM | 262 | OE1 | GLU | A | 50 | -8.357  | 43.957 | 9.988  | 1.000 | 46.50 |
| ATOM | 263 | OE2 | GLU | A | 50 | -6.639  | 43.930 | 8.604  | 1.000 | 70.90 |
| ATOM | 264 | C   | GLU | A | 50 | -6.238  | 41.369 | 13.861 | 1.000 | 25.23 |
| ATOM | 265 | O   | GLU | A | 50 | -7.375  | 41.121 | 14.248 | 1.000 | 30.99 |
| ATOM | 266 | N   | LEU | A | 51 | -5.239  | 40.508 | 13.957 | 1.000 | 26.01 |
| ATOM | 267 | CA  | LEU | A | 51 | -5.447  | 39.194 | 14.580 | 1.000 | 21.27 |
| ATOM | 268 | CB  | LEU | A | 51 | -4.470  | 38.237 | 13.898 | 1.000 | 22.16 |
| ATOM | 269 | CG  | LEU | A | 51 | -4.752  | 38.015 | 12.411 | 1.000 | 26.33 |
| ATOM | 270 | CD1 | LEU | A | 51 | -3.531  | 37.428 | 11.721 | 1.000 | 24.42 |
| ATOM | 271 | CD2 | LEU | A | 51 | -5.938  | 37.091 | 12.208 | 1.000 | 28.60 |
| ATOM | 272 | C   | LEU | A | 51 | -5.186  | 39.188 | 16.068 | 1.000 | 28.00 |
| ATOM | 273 | O   | LEU | A | 51 | -5.315  | 38.171 | 16.742 | 1.000 | 26.46 |
| ATOM | 274 | N   | LYS | A | 52 | -4.767  | 40.325 | 16.620 | 1.000 | 26.04 |
| ATOM | 275 | CA  | LYS | A | 52 | -4.297  | 40.372 | 18.002 | 1.000 | 27.42 |
| ATOM | 276 | CB  | LYS | A | 52 | -3.950  | 41.832 | 18.319 | 1.000 | 30.97 |
| ATOM | 277 | CG  | LYS | A | 52 | -3.602  | 42.133 | 19.765 | 1.000 | 36.67 |
| ATOM | 278 | CD  | LYS | A | 52 | -2.878  | 43.478 | 19.823 | 1.000 | 47.93 |
| ATOM | 279 | CE  | LYS | A | 52 | -3.089  | 44.186 | 21.148 | 1.000 | 54.43 |
| ATOM | 280 | NZ  | LYS | A | 52 | -3.831  | 45.481 | 20.963 | 1.000 | 76.91 |
| ATOM | 281 | C   | LYS | A | 52 | -5.281  | 39.803 | 19.009 | 1.000 | 30.56 |
| ATOM | 282 | O   | LYS | A | 52 | -4.866  | 38.997 | 19.848 | 1.000 | 31.78 |
| ATOM | 283 | N   | ASP | A | 53 | -6.560  | 40.166 | 18.951 | 1.000 | 22.00 |
| ATOM | 284 | CA  | ASP | A | 53 | -7.502  | 39.716 | 19.960 | 1.000 | 27.33 |
| ATOM | 285 | CB  | ASP | A | 53 | -8.442  | 40.858 | 20.385 | 1.000 | 30.10 |
| ATOM | 286 | CG  | ASP | A | 53 | -7.622  | 42.098 | 20.721 | 1.000 | 47.01 |
| ATOM | 287 | OD1 | ASP | A | 53 | -6.798  | 42.004 | 21.657 | 1.000 | 67.96 |
| ATOM | 288 | OD2 | ASP | A | 53 | -7.810  | 43.119 | 20.027 | 1.000 | 65.18 |
| ATOM | 289 | C   | ASP | A | 53 | -8.370  | 38.541 | 19.536 | 1.000 | 25.20 |
| ATOM | 290 | O   | ASP | A | 53 | -9.268  | 38.189 | 20.304 | 1.000 | 25.98 |
| ATOM | 291 | N   | VAL | A | 54 | -8.123  | 37.957 | 18.372 | 1.000 | 23.81 |
| ATOM | 292 | CA  | VAL | A | 54 | -8.897  | 36.770 | 17.995 | 1.000 | 20.94 |
| ATOM | 293 | CB  | VAL | A | 54 | -8.477  | 36.258 | 16.616 | 1.000 | 22.31 |
| ATOM | 294 | CG1 | VAL | A | 54 | -9.232  | 34.978 | 16.241 | 1.000 | 29.30 |
| ATOM | 295 | CG2 | VAL | A | 54 | -8.710  | 37.323 | 15.543 | 1.000 | 21.16 |
| ATOM | 296 | C   | VAL | A | 54 | -8.722  | 35.657 | 19.047 | 1.000 | 22.79 |
| ATOM | 297 | O   | VAL | A | 54 | -7.595  | 35.307 | 19.395 | 1.000 | 24.33 |
| ATOM | 298 | N   | GLY | A | 55 | -9.835  | 35.135 | 19.514 | 1.000 | 19.38 |
| ATOM | 299 | CA  | GLY | A | 55 | -10.013 | 34.105 | 20.496 | 1.000 | 21.67 |
| ATOM | 300 | C   | GLY | A | 55 | -9.849  | 34.607 | 21.923 | 1.000 | 26.11 |
| ATOM | 301 | O   | GLY | A | 55 | -10.150 | 33.822 | 22.828 | 1.000 | 24.18 |
| ATOM | 302 | N   | ARG | A | 56 | -9.400  | 35.842 | 22.115 | 1.000 | 28.14 |
| ATOM | 303 | CA  | ARG | A | 56 | -8.976  | 36.366 | 23.416 | 1.000 | 31.63 |
| ATOM | 304 | CB  | ARG | A | 56 | -8.162  | 37.661 | 23.262 | 1.000 | 32.19 |
| ATOM | 305 | CG  | ARG | A | 56 | -6.762  | 37.493 | 22.699 | 1.000 | 31.76 |
| ATOM | 306 | CD  | ARG | A | 56 | -5.957  | 36.532 | 23.528 | 1.000 | 29.57 |
| ATOM | 307 | NE  | ARG | A | 56 | -4.544  | 36.431 | 23.220 | 1.000 | 30.87 |
| ATOM | 308 | CZ  | ARG | A | 56 | -3.526  | 37.074 | 23.757 | 1.000 | 30.34 |
| ATOM | 309 | NH1 | ARG | A | 56 | -3.681  | 37.983 | 24.710 | 1.000 | 22.02 |
| ATOM | 310 | NH2 | ARG | A | 56 | -2.280  | 36.828 | 23.339 | 1.000 | 31.11 |
| ATOM | 311 | C   | ARG | A | 56 | -10.110 | 36.645 | 24.386 | 1.000 | 27.29 |

**FIGURE 207**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 312 | O   | ARG | A | 56 | -9.904  | 37.126 | 25.512 | 1.000 | 30.11 |
| ATOM | 313 | N   | ASN | A | 57 | -11.352 | 36.365 | 24.023 | 1.000 | 19.89 |
| ATOM | 314 | CA  | ASN | A | 57 | -12.429 | 36.544 | 24.990 | 1.000 | 21.90 |
| ATOM | 315 | CB  | ASN | A | 57 | -13.713 | 36.926 | 24.246 | 1.000 | 27.73 |
| ATOM | 316 | CG  | ASN | A | 57 | -14.041 | 35.852 | 23.214 | 1.000 | 36.94 |
| ATOM | 317 | OD1 | ASN | A | 57 | -13.158 | 35.389 | 22.486 | 1.000 | 42.61 |
| ATOM | 318 | ND2 | ASN | A | 57 | -15.303 | 35.449 | 23.148 | 1.000 | 39.27 |
| ATOM | 319 | C   | ASN | A | 57 | -12.594 | 35.274 | 25.807 | 1.000 | 27.58 |
| ATOM | 320 | O   | ASN | A | 57 | -13.336 | 35.218 | 26.785 | 1.000 | 32.05 |
| ATOM | 321 | N   | GLN | A | 58 | -11.917 | 34.193 | 25.434 | 1.000 | 25.93 |
| ATOM | 322 | CA  | GLN | A | 58 | -12.213 | 32.925 | 26.103 | 1.000 | 23.11 |
| ATOM | 323 | CB  | GLN | A | 58 | -11.975 | 31.773 | 25.109 | 1.000 | 24.51 |
| ATOM | 324 | CG  | GLN | A | 58 | -12.758 | 31.911 | 23.809 | 1.000 | 19.93 |
| ATOM | 325 | CD  | GLN | A | 58 | -12.245 | 30.977 | 22.712 | 1.000 | 21.00 |
| ATOM | 326 | OE1 | GLN | A | 58 | -11.224 | 31.206 | 22.055 | 1.000 | 21.51 |
| ATOM | 327 | NE2 | GLN | A | 58 | -12.953 | 29.879 | 22.484 | 1.000 | 21.23 |
| ATOM | 328 | C   | GLN | A | 58 | -11.396 | 32.695 | 27.366 | 1.000 | 23.30 |
| ATOM | 329 | O   | GLN | A | 58 | -10.242 | 33.132 | 27.462 | 1.000 | 24.27 |
| ATOM | 330 | N   | SER | A | 59 | -11.981 | 31.996 | 28.335 | 1.000 | 19.68 |
| ATOM | 331 | CA  | SER | A | 59 | -11.377 | 31.719 | 29.620 | 1.000 | 20.00 |
| ATOM | 332 | CB  | SER | A | 59 | -12.481 | 31.570 | 30.673 | 1.000 | 29.01 |
| ATOM | 333 | OG  | SER | A | 59 | -13.222 | 30.375 | 30.394 | 1.000 | 51.65 |
| ATOM | 334 | C   | SER | A | 59 | -10.565 | 30.423 | 29.617 | 1.000 | 32.69 |
| ATOM | 335 | O   | SER | A | 59 | -10.792 | 29.571 | 28.754 | 1.000 | 24.40 |
| ATOM | 336 | N   | CYS | A | 60 | -9.682  | 30.285 | 30.596 | 1.000 | 21.63 |
| ATOM | 337 | CA  | CYS | A | 60 | -8.872  | 29.128 | 30.861 | 1.000 | 19.92 |
| ATOM | 338 | CB  | CYS | A | 60 | -7.392  | 29.346 | 30.568 | 1.000 | 20.33 |
| ATOM | 339 | SG  | CYS | A | 60 | -7.068  | 30.023 | 28.934 | 1.000 | 23.64 |
| ATOM | 340 | C   | CYS | A | 60 | -8.980  | 28.736 | 32.344 | 1.000 | 21.45 |
| ATOM | 341 | O   | CYS | A | 60 | -7.941  | 28.497 | 32.959 | 1.000 | 20.03 |
| ATOM | 342 | N   | ASP | A | 61 | -10.220 | 28.697 | 32.804 | 1.000 | 22.24 |
| ATOM | 343 | CA  | ASP | A | 61 | -10.439 | 28.455 | 34.236 | 1.000 | 22.76 |
| ATOM | 344 | CB  | ASP | A | 61 | -11.912 | 28.676 | 34.545 | 1.000 | 26.65 |
| ATOM | 345 | CG  | ASP | A | 61 | -12.408 | 30.099 | 34.398 | 1.000 | 27.80 |
| ATOM | 346 | OD1 | ASP | A | 61 | -11.617 | 31.062 | 34.345 | 1.000 | 25.45 |
| ATOM | 347 | OD2 | ASP | A | 61 | -13.650 | 30.248 | 34.356 | 1.000 | 28.50 |
| ATOM | 348 | C   | ASP | A | 61 | -9.962  | 27.065 | 34.629 | 1.000 | 27.73 |
| ATOM | 349 | O   | ASP | A | 61 | -9.345  | 26.878 | 35.690 | 1.000 | 25.51 |
| ATOM | 350 | N   | ILE | A | 62 | -10.221 | 26.052 | 33.792 | 1.000 | 24.65 |
| ATOM | 351 | CA  | ILE | A | 62 | -9.809  | 24.698 | 34.223 | 1.000 | 21.14 |
| ATOM | 352 | CB  | ILE | A | 62 | -10.325 | 23.659 | 33.214 | 1.000 | 21.34 |
| ATOM | 353 | CG1 | ILE | A | 62 | -11.838 | 23.755 | 33.010 | 1.000 | 22.01 |
| ATOM | 354 | CD1 | ILE | A | 62 | -12.609 | 23.524 | 34.306 | 1.000 | 33.06 |
| ATOM | 355 | CG2 | ILE | A | 62 | -9.903  | 22.258 | 33.624 | 1.000 | 31.17 |
| ATOM | 356 | C   | ILE | A | 62 | -8.309  | 24.617 | 34.399 | 1.000 | 22.92 |
| ATOM | 357 | O   | ILE | A | 62 | -7.792  | 24.134 | 35.422 | 1.000 | 26.58 |
| ATOM | 358 | N   | ALA | A | 63 | -7.566  | 25.123 | 33.412 | 1.000 | 19.57 |
| ATOM | 359 | CA  | ALA | A | 63 | -6.122  | 25.164 | 33.470 | 1.000 | 19.70 |
| ATOM | 360 | CB  | ALA | A | 63 | -5.549  | 25.916 | 32.285 | 1.000 | 22.66 |
| ATOM | 361 | C   | ALA | A | 63 | -5.604  | 25.864 | 34.733 | 1.000 | 27.00 |
| ATOM | 362 | O   | ALA | A | 63 | -4.516  | 25.553 | 35.212 | 1.000 | 21.30 |
| ATOM | 363 | N   | LEU | A | 64 | -6.404  | 26.799 | 35.235 | 1.000 | 23.07 |

**FIGURE 208**

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 364 | CA  | LEU | A | 64 | -6.027  | 27.582 | 36.400 | 1.000 | 24.35 |
| ATOM | 365 | CB  | LEU | A | 64 | -6.749  | 28.929 | 36.297 | 1.000 | 23.45 |
| ATOM | 366 | CG  | LEU | A | 64 | -6.102  | 29.880 | 35.306 | 1.000 | 23.45 |
| ATOM | 367 | CD1 | LEU | A | 64 | -6.952  | 31.144 | 35.230 | 1.000 | 26.55 |
| ATOM | 368 | CD2 | LEU | A | 64 | -4.677  | 30.179 | 35.723 | 1.000 | 24.94 |
| ATOM | 369 | C   | LEU | A | 64 | -6.381  | 26.919 | 37.713 | 1.000 | 31.23 |
| ATOM | 370 | O   | LEU | A | 64 | -6.097  | 27.521 | 38.750 | 1.000 | 30.60 |
| ATOM | 371 | N   | LEU | A | 65 | -6.982  | 25.733 | 37.690 | 1.000 | 25.47 |
| ATOM | 372 | CA  | LEU | A | 65 | -7.306  | 25.047 | 38.937 | 1.000 | 27.75 |
| ATOM | 373 | CB  | LEU | A | 65 | -8.162  | 23.817 | 38.624 | 1.000 | 29.69 |
| ATOM | 374 | CG  | LEU | A | 65 | -9.587  | 24.168 | 38.169 | 1.000 | 29.27 |
| ATOM | 375 | CD1 | LEU | A | 65 | -10.317 | 22.915 | 37.710 | 1.000 | 22.91 |
| ATOM | 376 | CD2 | LEU | A | 65 | -10.326 | 24.875 | 39.294 | 1.000 | 45.21 |
| ATOM | 377 | C   | LEU | A | 65 | -6.045  | 24.666 | 39.697 | 1.000 | 32.88 |
| ATOM | 378 | O   | LEU | A | 65 | -5.049  | 24.217 | 39.140 | 1.000 | 35.70 |
| ATOM | 379 | N   | PRO | A | 66 | -6.075  | 24.876 | 41.014 | 1.000 | 36.18 |
| ATOM | 380 | CA  | PRO | A | 66 | -4.904  | 24.635 | 41.858 | 1.000 | 36.18 |
| ATOM | 381 | CB  | PRO | A | 66 | -5.488  | 24.754 | 43.275 | 1.000 | 47.92 |
| ATOM | 382 | CG  | PRO | A | 66 | -6.648  | 25.684 | 43.117 | 1.000 | 42.33 |
| ATOM | 383 | CD  | PRO | A | 66 | -7.235  | 25.378 | 41.764 | 1.000 | 30.77 |
| ATOM | 384 | C   | PRO | A | 66 | -4.302  | 23.248 | 41.658 | 1.000 | 26.18 |
| ATOM | 385 | O   | PRO | A | 66 | -3.084  | 23.122 | 41.569 | 1.000 | 37.38 |
| ATOM | 386 | N   | GLU | A | 67 | -5.151  | 22.242 | 41.580 | 1.000 | 33.07 |
| ATOM | 387 | CA  | GLU | A | 67 | -4.828  | 20.867 | 41.244 | 1.000 | 38.66 |
| ATOM | 388 | CB  | GLU | A | 67 | -6.138  | 20.071 | 41.150 | 1.000 | 40.47 |
| ATOM | 389 | CG  | GLU | A | 67 | -7.142  | 20.605 | 40.154 | 1.000 | 58.25 |
| ATOM | 390 | CD  | GLU | A | 67 | -8.530  | 20.002 | 40.228 | 1.000 | 70.71 |
| ATOM | 391 | OE1 | GLU | A | 67 | -8.874  | 19.134 | 39.390 | 1.000 | 47.20 |
| ATOM | 392 | OE2 | GLU | A | 67 | -9.311  | 20.406 | 41.123 | 1.000 | 81.59 |
| ATOM | 393 | C   | GLU | A | 67 | -4.033  | 20.762 | 39.946 | 1.000 | 40.21 |
| ATOM | 394 | O   | GLU | A | 67 | -3.232  | 19.837 | 39.768 | 1.000 | 33.36 |
| ATOM | 395 | N   | ASN | A | 68 | -4.202  | 21.695 | 39.001 | 1.000 | 27.60 |
| ATOM | 396 | CA  | ASN | A | 68 | -3.494  | 21.553 | 37.729 | 1.000 | 27.03 |
| ATOM | 397 | CB  | ASN | A | 68 | -4.471  | 21.891 | 36.584 | 1.000 | 25.75 |
| ATOM | 398 | CG  | ASN | A | 68 | -5.638  | 20.924 | 36.530 | 1.000 | 27.63 |
| ATOM | 399 | OD1 | ASN | A | 68 | -5.417  | 19.725 | 36.763 | 1.000 | 27.03 |
| ATOM | 400 | ND2 | ASN | A | 68 | -6.837  | 21.424 | 36.223 | 1.000 | 20.87 |
| ATOM | 401 | C   | ASN | A | 68 | -2.244  | 22.400 | 37.582 | 1.000 | 29.26 |
| ATOM | 402 | O   | ASN | A | 68 | -1.561  | 22.322 | 36.543 | 1.000 | 32.09 |
| ATOM | 403 | N   | ARG | A | 69 | -1.877  | 23.230 | 38.550 | 1.000 | 39.29 |
| ATOM | 404 | CA  | ARG | A | 69 | -0.765  | 24.169 | 38.333 | 1.000 | 36.83 |
| ATOM | 405 | CB  | ARG | A | 69 | -0.581  | 25.036 | 39.587 | 1.000 | 41.69 |
| ATOM | 406 | CG  | ARG | A | 69 | 0.072   | 26.376 | 39.290 | 1.000 | 44.04 |
| ATOM | 407 | CD  | ARG | A | 69 | -0.117  | 27.331 | 40.461 | 1.000 | 60.35 |
| ATOM | 408 | NE  | ARG | A | 69 | -1.481  | 27.376 | 40.972 | 1.000 | 61.46 |
| ATOM | 409 | CZ  | ARG | A | 69 | -1.832  | 27.284 | 42.248 | 1.000 | 67.83 |
| ATOM | 410 | NH1 | ARG | A | 69 | -3.113  | 27.336 | 42.599 | 1.000 | 61.15 |
| ATOM | 411 | NH2 | ARG | A | 69 | -0.920  | 27.136 | 43.202 | 1.000 | 84.01 |
| ATOM | 412 | C   | ARG | A | 69 | 0.541   | 23.491 | 37.948 | 1.000 | 31.02 |
| ATOM | 413 | O   | ARG | A | 69 | 1.225   | 23.924 | 37.009 | 1.000 | 34.71 |
| ATOM | 414 | N   | GLY | A | 70 | 0.895   | 22.385 | 38.603 | 1.000 | 27.71 |
| ATOM | 415 | CA  | GLY | A | 70 | 2.103   | 21.679 | 38.203 | 1.000 | 25.00 |

**FIGURE 209**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |       |       |
|------|-----|-----|-----|---|----|--------|--------|--------|-------|-------|
| ATOM | 416 | C   | GLY | A | 70 | 2.044  | 21.041 | 36.822 | 1.000 | 24.89 |
| ATOM | 417 | O   | GLY | A | 70 | 3.083  | 20.564 | 36.376 | 1.000 | 31.72 |
| ATOM | 418 | N   | LYS | A | 71 | 0.903  | 21.014 | 36.147 | 1.000 | 27.08 |
| ATOM | 419 | CA  | LYS | A | 71 | 0.763  | 20.318 | 34.866 | 1.000 | 24.21 |
| ATOM | 420 | CB  | LYS | A | 71 | -0.653 | 19.731 | 34.781 | 1.000 | 21.70 |
| ATOM | 421 | CG  | LYS | A | 71 | -0.943 | 18.621 | 35.788 | 1.000 | 25.95 |
| ATOM | 422 | CD  | LYS | A | 71 | -2.404 | 18.202 | 35.750 | 1.000 | 27.35 |
| ATOM | 423 | CE  | LYS | A | 71 | -2.743 | 17.164 | 36.834 | 1.000 | 26.32 |
| ATOM | 424 | NZ  | LYS | A | 71 | -4.227 | 17.045 | 36.994 | 1.000 | 29.99 |
| ATOM | 425 | C   | LYS | A | 71 | 1.003  | 21.230 | 33.678 | 1.000 | 26.31 |
| ATOM | 426 | O   | LYS | A | 71 | 0.999  | 20.826 | 32.508 | 1.000 | 21.01 |
| ATOM | 427 | N   | ASN | A | 72 | 1.209  | 22.517 | 33.974 | 1.000 | 24.08 |
| ATOM | 428 | CA  | ASN | A | 72 | 1.520  | 23.503 | 32.951 | 1.000 | 24.06 |
| ATOM | 429 | CB  | ASN | A | 72 | 0.700  | 24.782 | 33.236 | 1.000 | 23.98 |
| ATOM | 430 | CG  | ASN | A | 72 | -0.782 | 24.508 | 33.170 | 1.000 | 24.00 |
| ATOM | 431 | OD1 | ASN | A | 72 | -1.229 | 23.905 | 32.180 | 1.000 | 27.29 |
| ATOM | 432 | ND2 | ASN | A | 72 | -1.564 | 24.932 | 34.139 | 1.000 | 21.52 |
| ATOM | 433 | C   | ASN | A | 72 | 2.999  | 23.855 | 32.902 | 1.000 | 24.14 |
| ATOM | 434 | O   | ASN | A | 72 | 3.539  | 24.242 | 33.952 | 1.000 | 32.17 |
| ATOM | 435 | N   | ARG | A | 73 | 3.669  | 23.767 | 31.763 | 1.000 | 18.37 |
| ATOM | 436 | CA  | ARG | A | 73 | 5.068  | 24.153 | 31.624 | 1.000 | 20.26 |
| ATOM | 437 | CB  | ARG | A | 73 | 5.606  | 23.824 | 30.236 | 1.000 | 27.07 |
| ATOM | 438 | CG  | ARG | A | 73 | 7.082  | 24.137 | 30.020 | 1.000 | 24.27 |
| ATOM | 439 | CD  | ARG | A | 73 | 7.645  | 23.603 | 28.712 | 1.000 | 22.01 |
| ATOM | 440 | NE  | ARG | A | 73 | 7.794  | 22.144 | 28.739 | 1.000 | 23.84 |
| ATOM | 441 | CZ  | ARG | A | 73 | 8.809  | 21.516 | 29.321 | 1.000 | 33.27 |
| ATOM | 442 | NH1 | ARG | A | 73 | 9.757  | 22.240 | 29.913 | 1.000 | 21.92 |
| ATOM | 443 | NH2 | ARG | A | 73 | 8.909  | 20.191 | 29.335 | 1.000 | 23.01 |
| ATOM | 444 | C   | ARG | A | 73 | 5.231  | 25.648 | 31.916 | 1.000 | 30.65 |
| ATOM | 445 | O   | ARG | A | 73 | 6.184  | 26.110 | 32.549 | 1.000 | 32.85 |
| ATOM | 446 | N   | TYR | A | 74 | 4.279  | 26.440 | 31.452 | 1.000 | 27.96 |
| ATOM | 447 | CA  | TYR | A | 74 | 4.329  | 27.903 | 31.619 | 1.000 | 22.72 |
| ATOM | 448 | CB  | TYR | A | 74 | 4.778  | 28.577 | 30.343 | 1.000 | 24.68 |
| ATOM | 449 | CG  | TYR | A | 74 | 6.008  | 28.085 | 29.620 | 1.000 | 40.81 |
| ATOM | 450 | CD1 | TYR | A | 74 | 7.302  | 28.339 | 30.080 | 1.000 | 42.06 |
| ATOM | 451 | CE1 | TYR | A | 74 | 8.424  | 27.881 | 29.404 | 1.000 | 30.31 |
| ATOM | 452 | CZ  | TYR | A | 74 | 8.304  | 27.155 | 28.238 | 1.000 | 36.98 |
| ATOM | 453 | OH  | TYR | A | 74 | 9.426  | 26.707 | 27.567 | 1.000 | 31.11 |
| ATOM | 454 | CE2 | TYR | A | 74 | 7.038  | 26.881 | 27.739 | 1.000 | 33.48 |
| ATOM | 455 | CD2 | TYR | A | 74 | 5.932  | 27.349 | 28.434 | 1.000 | 32.64 |
| ATOM | 456 | C   | TYR | A | 74 | 2.932  | 28.320 | 32.074 | 1.000 | 35.24 |
| ATOM | 457 | O   | TYR | A | 74 | 1.980  | 28.127 | 31.311 | 1.000 | 28.99 |
| ATOM | 458 | N   | ASN | A | 75 | 2.831  | 28.838 | 33.293 | 1.000 | 34.47 |
| ATOM | 459 | CA  | ASN | A | 75 | 1.587  | 29.142 | 33.973 | 1.000 | 26.33 |
| ATOM | 460 | CB  | ASN | A | 75 | 1.844  | 29.654 | 35.396 | 1.000 | 28.02 |
| ATOM | 461 | CG  | ASN | A | 75 | 2.541  | 28.595 | 36.230 | 1.000 | 47.27 |
| ATOM | 462 | OD1 | ASN | A | 75 | 2.639  | 27.427 | 35.838 | 1.000 | 38.13 |
| ATOM | 463 | ND2 | ASN | A | 75 | 3.009  | 29.045 | 37.388 | 1.000 | 58.84 |
| ATOM | 464 | C   | ASN | A | 75 | 0.752  | 30.193 | 33.247 | 1.000 | 19.13 |
| ATOM | 465 | O   | ASN | A | 75 | -0.423 | 30.394 | 33.561 | 1.000 | 27.32 |
| ATOM | 466 | N   | ASN | A | 76 | 1.348  | 30.876 | 32.289 | 1.000 | 18.49 |
| ATOM | 467 | CA  | ASN | A | 76 | 0.562  | 31.826 | 31.510 | 1.000 | 26.54 |

**FIGURE 210**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 468 | CB  | ASN | A | 76 | 1.244   | 33.195 | 31.432 | 1.000 | 26.00 |
| ATOM | 469 | CG  | ASN | A | 76 | 2.628   | 33.130 | 30.821 | 1.000 | 27.59 |
| ATOM | 470 | OD1 | ASN | A | 76 | 3.295   | 32.100 | 30.926 | 1.000 | 28.39 |
| ATOM | 471 | ND2 | ASN | A | 76 | 3.131   | 34.186 | 30.182 | 1.000 | 26.81 |
| ATOM | 472 | C   | ASN | A | 76 | 0.331   | 31.297 | 30.101 | 1.000 | 26.92 |
| ATOM | 473 | O   | ASN | A | 76 | -0.145  | 32.065 | 29.263 | 1.000 | 24.80 |
| ATOM | 474 | N   | ILE | A | 77 | 0.659   | 30.023 | 29.813 | 1.000 | 21.21 |
| ATOM | 475 | CA  | ILE | A | 77 | 0.313   | 29.527 | 28.477 | 1.000 | 20.79 |
| ATOM | 476 | CB  | ILE | A | 77 | 1.534   | 29.187 | 27.632 | 1.000 | 25.15 |
| ATOM | 477 | CG1 | ILE | A | 77 | 2.596   | 30.315 | 27.595 | 1.000 | 31.48 |
| ATOM | 478 | CD1 | ILE | A | 77 | 2.862   | 30.817 | 26.195 | 1.000 | 49.78 |
| ATOM | 479 | CG2 | ILE | A | 77 | 1.116   | 28.793 | 26.229 | 1.000 | 23.01 |
| ATOM | 480 | C   | ILE | A | 77 | -0.604  | 28.313 | 28.648 | 1.000 | 23.40 |
| ATOM | 481 | O   | ILE | A | 77 | -0.121  | 27.210 | 28.877 | 1.000 | 24.16 |
| ATOM | 482 | N   | LEU | A | 78 | -1.899  | 28.584 | 28.583 | 1.000 | 20.25 |
| ATOM | 483 | CA  | LEU | A | 78 | -2.931  | 27.667 | 29.035 | 1.000 | 19.58 |
| ATOM | 484 | CB  | LEU | A | 78 | -3.621  | 28.170 | 30.307 | 1.000 | 18.02 |
| ATOM | 485 | CG  | LEU | A | 78 | -2.711  | 28.581 | 31.476 | 1.000 | 22.60 |
| ATOM | 486 | CD1 | LEU | A | 78 | -3.510  | 29.136 | 32.647 | 1.000 | 18.50 |
| ATOM | 487 | CD2 | LEU | A | 78 | -1.854  | 27.424 | 31.993 | 1.000 | 19.12 |
| ATOM | 488 | C   | LEU | A | 78 | -3.946  | 27.471 | 27.912 | 1.000 | 18.12 |
| ATOM | 489 | O   | LEU | A | 78 | -4.186  | 28.398 | 27.142 | 1.000 | 19.00 |
| ATOM | 490 | N   | PRO | A | 79 | -4.511  | 26.269 | 27.863 | 1.000 | 18.26 |
| ATOM | 491 | CA  | PRO | A | 79 | -5.546  | 26.003 | 26.858 | 1.000 | 16.50 |
| ATOM | 492 | CB  | PRO | A | 79 | -5.707  | 24.485 | 26.984 | 1.000 | 21.55 |
| ATOM | 493 | CG  | PRO | A | 79 | -5.462  | 24.228 | 28.452 | 1.000 | 13.29 |
| ATOM | 494 | CD  | PRO | A | 79 | -4.246  | 25.103 | 28.705 | 1.000 | 14.71 |
| ATOM | 495 | C   | PRO | A | 79 | -6.844  | 26.703 | 27.235 | 1.000 | 17.47 |
| ATOM | 496 | O   | PRO | A | 79 | -7.176  | 26.850 | 28.420 | 1.000 | 20.15 |
| ATOM | 497 | N   | TYR | A | 80 | -7.613  | 27.139 | 26.237 | 1.000 | 15.99 |
| ATOM | 498 | CA  | TYR | A | 80 | -8.958  | 27.654 | 26.481 | 1.000 | 17.04 |
| ATOM | 499 | CB  | TYR | A | 80 | -9.454  | 28.253 | 25.165 | 1.000 | 16.02 |
| ATOM | 500 | CG  | TYR | A | 80 | -8.756  | 29.502 | 24.697 | 1.000 | 17.83 |
| ATOM | 501 | CD1 | TYR | A | 80 | -8.514  | 30.562 | 25.574 | 1.000 | 17.44 |
| ATOM | 502 | CE1 | TYR | A | 80 | -7.879  | 31.711 | 25.143 | 1.000 | 18.38 |
| ATOM | 503 | CZ  | TYR | A | 80 | -7.474  | 31.828 | 23.837 | 1.000 | 17.97 |
| ATOM | 504 | OH  | TYR | A | 80 | -6.845  | 32.976 | 23.415 | 1.000 | 20.65 |
| ATOM | 505 | CE2 | TYR | A | 80 | -7.700  | 30.802 | 22.930 | 1.000 | 19.84 |
| ATOM | 506 | CD2 | TYR | A | 80 | -8.338  | 29.655 | 23.381 | 1.000 | 17.33 |
| ATOM | 507 | C   | TYR | A | 80 | -9.884  | 26.547 | 26.977 | 1.000 | 18.38 |
| ATOM | 508 | O   | TYR | A | 80 | -9.791  | 25.404 | 26.525 | 1.000 | 19.85 |
| ATOM | 509 | N   | ASP | A | 81 | -10.785 | 26.816 | 27.908 | 1.000 | 18.35 |
| ATOM | 510 | CA  | ASP | A | 81 | -11.772 | 25.824 | 28.336 | 1.000 | 23.15 |
| ATOM | 511 | CB  | ASP | A | 81 | -12.734 | 26.485 | 29.337 | 1.000 | 20.21 |
| ATOM | 512 | CG  | ASP | A | 81 | -12.050 | 26.883 | 30.626 | 1.000 | 19.62 |
| ATOM | 513 | OD1 | ASP | A | 81 | -11.107 | 26.212 | 31.082 | 1.000 | 20.36 |
| ATOM | 514 | OD2 | ASP | A | 81 | -12.437 | 27.911 | 31.225 | 1.000 | 24.76 |
| ATOM | 515 | C   | ASP | A | 81 | -12.539 | 25.250 | 27.153 | 1.000 | 19.52 |
| ATOM | 516 | O   | ASP | A | 81 | -12.771 | 24.029 | 27.079 | 1.000 | 21.17 |
| ATOM | 517 | N   | ALA | A | 82 | -12.910 | 26.116 | 26.218 | 1.000 | 19.35 |
| ATOM | 518 | CA  | ALA | A | 82 | -13.787 | 25.780 | 25.106 | 1.000 | 20.79 |
| ATOM | 519 | CB  | ALA | A | 82 | -14.147 | 27.041 | 24.318 | 1.000 | 21.73 |

**FIGURE 211**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |       |       |
|------|-----|-----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 520 | C   | ALA | A | 82 | -13.218 | 24.780 | 24.117 | 1.000 | 24.48 |
| ATOM | 521 | O   | ALA | A | 82 | -14.017 | 24.152 | 23.409 | 1.000 | 24.01 |
| ATOM | 522 | N   | THR | A | 83 | -11.910 | 24.613 | 24.002 | 1.000 | 19.51 |
| ATOM | 523 | CA  | THR | A | 83 | -11.324 | 23.717 | 22.995 | 1.000 | 17.80 |
| ATOM | 524 | CB  | THR | A | 83 | -10.631 | 24.588 | 21.940 | 1.000 | 16.46 |
| ATOM | 525 | OG1 | THR | A | 83 | -9.691  | 25.412 | 22.665 | 1.000 | 18.46 |
| ATOM | 526 | CG2 | THR | A | 83 | -11.616 | 25.512 | 21.246 | 1.000 | 23.15 |
| ATOM | 527 | C   | THR | A | 83 | -10.302 | 22.753 | 23.586 | 1.000 | 19.19 |
| ATOM | 528 | O   | THR | A | 83 | -9.519  | 22.101 | 22.875 | 1.000 | 18.99 |
| ATOM | 529 | N   | ARG | A | 84 | -10.239 | 22.638 | 24.919 | 1.000 | 15.87 |
| ATOM | 530 | CA  | ARG | A | 84 | -9.214  | 21.790 | 25.521 | 1.000 | 13.38 |
| ATOM | 531 | CB  | ARG | A | 84 | -9.125  | 22.053 | 27.033 | 1.000 | 17.35 |
| ATOM | 532 | CG  | ARG | A | 84 | -10.272 | 21.451 | 27.842 | 1.000 | 15.57 |
| ATOM | 533 | CD  | ARG | A | 84 | -10.161 | 21.906 | 29.303 | 1.000 | 23.22 |
| ATOM | 534 | NE  | ARG | A | 84 | -11.142 | 21.257 | 30.168 | 1.000 | 23.41 |
| ATOM | 535 | CZ  | ARG | A | 84 | -10.962 | 20.204 | 30.948 | 1.000 | 20.47 |
| ATOM | 536 | NH1 | ARG | A | 84 | -9.809  | 19.561 | 31.054 | 1.000 | 19.35 |
| ATOM | 537 | NH2 | ARG | A | 84 | -11.994 | 19.773 | 31.664 | 1.000 | 22.12 |
| ATOM | 538 | C   | ARG | A | 84 | -9.470  | 20.299 | 25.308 | 1.000 | 18.88 |
| ATOM | 539 | O   | ARG | A | 84 | -10.635 | 19.874 | 25.268 | 1.000 | 22.06 |
| ATOM | 540 | N   | VAL | A | 85 | -8.375  | 19.551 | 25.196 | 1.000 | 16.89 |
| ATOM | 541 | CA  | VAL | A | 85 | -8.423  | 18.097 | 25.114 | 1.000 | 16.58 |
| ATOM | 542 | CB  | VAL | A | 85 | -7.184  | 17.483 | 24.455 | 1.000 | 22.94 |
| ATOM | 543 | CG1 | VAL | A | 85 | -7.356  | 15.966 | 24.274 | 1.000 | 23.40 |
| ATOM | 544 | CG2 | VAL | A | 85 | -6.893  | 18.086 | 23.091 | 1.000 | 17.65 |
| ATOM | 545 | C   | VAL | A | 85 | -8.595  | 17.535 | 26.523 | 1.000 | 19.64 |
| ATOM | 546 | O   | VAL | A | 85 | -7.844  | 17.914 | 27.424 | 1.000 | 19.96 |
| ATOM | 547 | N   | LYS | A | 86 | -9.550  | 16.650 | 26.756 | 1.000 | 17.33 |
| ATOM | 548 | CA  | LYS | A | 86 | -9.719  | 16.095 | 28.096 | 1.000 | 23.43 |
| ATOM | 549 | CB  | LYS | A | 86 | -11.191 | 16.082 | 28.526 | 1.000 | 27.56 |
| ATOM | 550 | CG  | LYS | A | 86 | -11.884 | 17.432 | 28.490 | 1.000 | 32.74 |
| ATOM | 551 | CD  | LYS | A | 86 | -13.319 | 17.288 | 28.987 | 1.000 | 42.78 |
| ATOM | 552 | CE  | LYS | A | 86 | -14.275 | 18.120 | 28.145 | 1.000 | 53.05 |
| ATOM | 553 | NZ  | LYS | A | 86 | -14.205 | 19.569 | 28.476 | 1.000 | 47.90 |
| ATOM | 554 | C   | LYS | A | 86 | -9.213  | 14.660 | 28.171 | 1.000 | 23.69 |
| ATOM | 555 | O   | LYS | A | 86 | -9.417  | 13.887 | 27.241 | 1.000 | 24.18 |
| ATOM | 556 | N   | LEU | A | 87 | -8.580  | 14.294 | 29.273 | 1.000 | 21.05 |
| ATOM | 557 | CA  | LEU | A | 87 | -8.225  | 12.906 | 29.504 | 1.000 | 18.28 |
| ATOM | 558 | CB  | LEU | A | 87 | -7.106  | 12.861 | 30.540 | 1.000 | 19.01 |
| ATOM | 559 | CG  | LEU | A | 87 | -5.824  | 13.608 | 30.146 | 1.000 | 24.48 |
| ATOM | 560 | CD1 | LEU | A | 87 | -4.865  | 13.612 | 31.326 | 1.000 | 21.86 |
| ATOM | 561 | CD2 | LEU | A | 87 | -5.175  | 12.994 | 28.916 | 1.000 | 21.83 |
| ATOM | 562 | C   | LEU | A | 87 | -9.433  | 12.132 | 30.001 | 1.000 | 30.80 |
| ATOM | 563 | O   | LEU | A | 87 | -10.293 | 12.739 | 30.652 | 1.000 | 27.84 |
| ATOM | 564 | N   | SER | A | 88 | -9.561  | 10.832 | 29.745 | 1.000 | 25.76 |
| ATOM | 565 | CA  | SER | A | 88 | -10.662 | 10.132 | 30.429 | 1.000 | 30.68 |
| ATOM | 566 | CB  | SER | A | 88 | -10.751 | 8.668  | 29.990 | 1.000 | 25.39 |
| ATOM | 567 | OG  | SER | A | 88 | -9.581  | 7.992  | 30.416 | 1.000 | 28.79 |
| ATOM | 568 | C   | SER | A | 88 | -10.554 | 10.163 | 31.955 | 1.000 | 34.04 |
| ATOM | 569 | O   | SER | A | 88 | -9.497  | 10.278 | 32.577 | 1.000 | 30.33 |
| ATOM | 570 | N   | ASN | A | 89 | -11.728 | 10.055 | 32.566 | 1.000 | 43.34 |
| ATOM | 571 | CA  | ASN | A | 89 | -11.976 | 10.144 | 33.991 | 1.000 | 56.50 |

**FIGURE 212**



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|      |     |     |     |   |     |         |        |        |       |       |
|------|-----|-----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 572 | CB  | ASN | A | 89  | -13.369 | 9.595  | 34.329 | 1.000 | 60.50 |
| ATOM | 573 | CG  | ASN | A | 89  | -13.557 | 8.127  | 34.024 | 1.000 | 66.77 |
| ATOM | 574 | OD1 | ASN | A | 89  | -12.606 | 7.351  | 33.952 | 1.000 | 60.44 |
| ATOM | 575 | ND2 | ASN | A | 89  | -14.807 | 7.703  | 33.844 | 1.000 | 70.97 |
| ATOM | 576 | C   | ASN | A | 89  | -10.926 | 9.410  | 34.821 | 1.000 | 65.63 |
| ATOM | 577 | O   | ASN | A | 89  | -10.996 | 9.390  | 36.052 | 1.000 | 72.13 |
| ATOM | 578 | N   | SER | A | 96  | -8.513  | 15.291 | 37.171 | 1.000 | 39.19 |
| ATOM | 579 | CA  | SER | A | 96  | -7.743  | 14.211 | 36.560 | 1.000 | 29.84 |
| ATOM | 580 | CB  | SER | A | 96  | -8.043  | 12.853 | 37.183 | 1.000 | 29.33 |
| ATOM | 581 | OG  | SER | A | 96  | -9.336  | 12.376 | 36.866 | 1.000 | 31.86 |
| ATOM | 582 | C   | SER | A | 96  | -7.971  | 14.200 | 35.049 | 1.000 | 25.03 |
| ATOM | 583 | O   | SER | A | 96  | -7.285  | 13.420 | 34.378 | 1.000 | 30.76 |
| ATOM | 584 | N   | ASP | A | 97  | -8.874  | 15.033 | 34.527 | 1.000 | 26.35 |
| ATOM | 585 | CA  | ASP | A | 97  | -9.072  | 15.047 | 33.069 | 1.000 | 23.38 |
| ATOM | 586 | CB  | ASP | A | 97  | -10.495 | 15.418 | 32.661 | 1.000 | 21.60 |
| ATOM | 587 | CG  | ASP | A | 97  | -10.928 | 16.834 | 32.933 | 1.000 | 26.73 |
| ATOM | 588 | OD1 | ASP | A | 97  | -10.115 | 17.686 | 33.354 | 1.000 | 26.07 |
| ATOM | 589 | OD2 | ASP | A | 97  | -12.136 | 17.107 | 32.701 | 1.000 | 29.59 |
| ATOM | 590 | C   | ASP | A | 97  | -8.112  | 16.015 | 32.379 | 1.000 | 28.59 |
| ATOM | 591 | O   | ASP | A | 97  | -8.144  | 16.087 | 31.149 | 1.000 | 22.81 |
| ATOM | 592 | N   | TYR | A | 98  | -7.316  | 16.753 | 33.150 | 1.000 | 24.51 |
| ATOM | 593 | CA  | TYR | A | 98  | -6.573  | 17.864 | 32.576 | 1.000 | 18.45 |
| ATOM | 594 | CB  | TYR | A | 98  | -6.287  | 18.947 | 33.663 | 1.000 | 21.47 |
| ATOM | 595 | CG  | TYR | A | 98  | -5.566  | 20.114 | 33.013 | 1.000 | 18.45 |
| ATOM | 596 | CD1 | TYR | A | 98  | -6.288  | 21.015 | 32.223 | 1.000 | 20.80 |
| ATOM | 597 | CE1 | TYR | A | 98  | -5.651  | 22.093 | 31.617 | 1.000 | 19.85 |
| ATOM | 598 | CZ  | TYR | A | 98  | -4.300  | 22.277 | 31.775 | 1.000 | 20.41 |
| ATOM | 599 | OH  | TYR | A | 98  | -3.617  | 23.313 | 31.194 | 1.000 | 18.24 |
| ATOM | 600 | CE2 | TYR | A | 98  | -3.554  | 21.399 | 32.546 | 1.000 | 19.23 |
| ATOM | 601 | CD2 | TYR | A | 98  | -4.206  | 20.342 | 33.147 | 1.000 | 19.12 |
| ATOM | 602 | C   | TYR | A | 98  | -5.263  | 17.498 | 31.918 | 1.000 | 19.64 |
| ATOM | 603 | O   | TYR | A | 98  | -4.369  | 16.840 | 32.439 | 1.000 | 20.66 |
| ATOM | 604 | N   | ILE | A | 99  | -5.119  | 18.053 | 30.711 | 1.000 | 16.91 |
| ATOM | 605 | CA  | ILE | A | 99  | -3.822  | 18.176 | 30.062 | 1.000 | 16.84 |
| ATOM | 606 | CB  | ILE | A | 99  | -3.536  | 17.002 | 29.113 | 1.000 | 17.82 |
| ATOM | 607 | CG1 | ILE | A | 99  | -2.137  | 16.977 | 28.518 | 1.000 | 15.01 |
| ATOM | 608 | CD1 | ILE | A | 99  | -1.789  | 15.688 | 27.785 | 1.000 | 15.78 |
| ATOM | 609 | CG2 | ILE | A | 99  | -4.615  | 16.953 | 28.023 | 1.000 | 17.57 |
| ATOM | 610 | C   | ILE | A | 99  | -3.766  | 19.520 | 29.325 | 1.000 | 15.16 |
| ATOM | 611 | O   | ILE | A | 99  | -4.767  | 20.020 | 28.812 | 1.000 | 17.38 |
| ATOM | 612 | N   | ASN | A | 100 | -2.587  | 20.120 | 29.308 | 1.000 | 17.52 |
| ATOM | 613 | CA  | ASN | A | 100 | -2.392  | 21.383 | 28.584 | 1.000 | 13.18 |
| ATOM | 614 | CB  | ASN | A | 100 | -1.125  | 22.085 | 29.028 | 1.000 | 14.04 |
| ATOM | 615 | CG  | ASN | A | 100 | -1.059  | 23.494 | 28.450 | 1.000 | 15.18 |
| ATOM | 616 | OD1 | ASN | A | 100 | -1.331  | 23.713 | 27.280 | 1.000 | 18.72 |
| ATOM | 617 | ND2 | ASN | A | 100 | -0.702  | 24.455 | 29.274 | 1.000 | 16.16 |
| ATOM | 618 | C   | ASN | A | 100 | -2.333  | 21.054 | 27.090 | 1.000 | 12.55 |
| ATOM | 619 | O   | ASN | A | 100 | -1.244  | 20.809 | 26.544 | 1.000 | 15.92 |
| ATOM | 620 | N   | ALA | A | 101 | -3.521  | 21.008 | 26.492 | 1.000 | 15.34 |
| ATOM | 621 | CA  | ALA | A | 101 | -3.655  | 20.605 | 25.088 | 1.000 | 18.55 |
| ATOM | 622 | CB  | ALA | A | 101 | -3.556  | 19.090 | 24.924 | 1.000 | 16.55 |
| ATOM | 623 | C   | ALA | A | 101 | -4.971  | 21.137 | 24.527 | 1.000 | 13.59 |

**FIGURE 213**

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|      |     |     |     |   |     |         |        |        |       |       |
|------|-----|-----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 624 | O   | ALA | A | 101 | -5.924  | 21.365 | 25.274 | 1.000 | 16.49 |
| ATOM | 625 | N   | SER | A | 102 | -5.001  | 21.341 | 23.211 | 1.000 | 13.49 |
| ATOM | 626 | CA  | SER | A | 102 | -6.108  | 21.993 | 22.553 | 1.000 | 16.27 |
| ATOM | 627 | CB  | SER | A | 102 | -5.855  | 23.491 | 22.338 | 1.000 | 21.21 |
| ATOM | 628 | OG  | SER | A | 102 | -5.352  | 24.131 | 23.503 | 1.000 | 17.32 |
| ATOM | 629 | C   | SER | A | 102 | -6.356  | 21.367 | 21.169 | 1.000 | 14.55 |
| ATOM | 630 | O   | SER | A | 102 | -5.410  | 21.018 | 20.464 | 1.000 | 15.20 |
| ATOM | 631 | N   | TYR | A | 103 | -7.636  | 21.254 | 20.835 | 1.000 | 16.64 |
| ATOM | 632 | CA  | TYR | A | 103 | -8.048  | 20.802 | 19.512 | 1.000 | 14.77 |
| ATOM | 633 | CB  | TYR | A | 103 | -9.467  | 20.239 | 19.531 | 1.000 | 18.66 |
| ATOM | 634 | CG  | TYR | A | 103 | -9.703  | 18.944 | 20.270 | 1.000 | 18.68 |
| ATOM | 635 | CD1 | TYR | A | 103 | -9.140  | 17.745 | 19.852 | 1.000 | 16.61 |
| ATOM | 636 | CE1 | TYR | A | 103 | -9.358  | 16.546 | 20.528 | 1.000 | 17.11 |
| ATOM | 637 | CZ  | TYR | A | 103 | -10.159 | 16.548 | 21.648 | 1.000 | 20.45 |
| ATOM | 638 | OH  | TYR | A | 103 | -10.386 | 15.378 | 22.329 | 1.000 | 23.33 |
| ATOM | 639 | CE2 | TYR | A | 103 | -10.730 | 17.732 | 22.079 | 1.000 | 22.73 |
| ATOM | 640 | CD2 | TYR | A | 103 | -10.517 | 18.922 | 21.410 | 1.000 | 19.22 |
| ATOM | 641 | C   | TYR | A | 103 | -7.987  | 21.941 | 18.505 | 1.000 | 13.95 |
| ATOM | 642 | O   | TYR | A | 103 | -8.391  | 23.073 | 18.745 | 1.000 | 19.80 |
| ATOM | 643 | N   | ILE | A | 104 | -7.482  | 21.618 | 17.316 | 1.000 | 18.42 |
| ATOM | 644 | CA  | ILE | A | 104 | -7.360  | 22.569 | 16.229 | 1.000 | 18.12 |
| ATOM | 645 | CB  | ILE | A | 104 | -5.872  | 22.884 | 15.979 | 1.000 | 23.14 |
| ATOM | 646 | CG1 | ILE | A | 104 | -5.070  | 23.233 | 17.226 | 1.000 | 28.92 |
| ATOM | 647 | CD1 | ILE | A | 104 | -5.524  | 24.493 | 17.940 | 1.000 | 29.26 |
| ATOM | 648 | CG2 | ILE | A | 104 | -5.741  | 24.005 | 14.967 | 1.000 | 26.42 |
| ATOM | 649 | C   | ILE | A | 104 | -7.946  | 22.001 | 14.952 | 1.000 | 23.75 |
| ATOM | 650 | O   | ILE | A | 104 | -7.672  | 20.852 | 14.601 | 1.000 | 21.79 |
| ATOM | 651 | N   | PRO | A | 105 | -8.754  | 22.779 | 14.241 | 1.000 | 28.20 |
| ATOM | 652 | CA  | PRO | A | 105 | -9.258  | 22.365 | 12.917 | 1.000 | 23.95 |
| ATOM | 653 | CB  | PRO | A | 105 | -10.391 | 23.355 | 12.645 | 1.000 | 31.38 |
| ATOM | 654 | CG  | PRO | A | 105 | -10.630 | 24.049 | 13.941 | 1.000 | 40.77 |
| ATOM | 655 | CD  | PRO | A | 105 | -9.285  | 24.093 | 14.643 | 1.000 | 28.64 |
| ATOM | 656 | C   | PRO | A | 105 | -8.174  | 22.464 | 11.860 | 1.000 | 28.29 |
| ATOM | 657 | O   | PRO | A | 105 | -7.183  | 23.199 | 11.926 | 1.000 | 24.10 |
| ATOM | 658 | N   | GLY | A | 106 | -8.320  | 21.674 | 10.798 | 1.000 | 25.13 |
| ATOM | 659 | CA  | GLY | A | 106 | -7.343  | 21.757 | 9.710  | 1.000 | 22.26 |
| ATOM | 660 | C   | GLY | A | 106 | -8.127  | 21.803 | 8.403  | 1.000 | 28.91 |
| ATOM | 661 | O   | GLY | A | 106 | -9.318  | 22.118 | 8.467  | 1.000 | 26.90 |
| ATOM | 662 | N   | ASN | A | 107 | -7.481  | 21.487 | 7.285  | 1.000 | 25.90 |
| ATOM | 663 | CA  | ASN | A | 107 | -8.184  | 21.653 | 6.010  | 1.000 | 35.70 |
| ATOM | 664 | CB  | ASN | A | 107 | -7.264  | 21.551 | 4.794  | 1.000 | 32.05 |
| ATOM | 665 | CG  | ASN | A | 107 | -6.326  | 22.729 | 4.615  | 1.000 | 27.43 |
| ATOM | 666 | OD1 | ASN | A | 107 | -5.615  | 22.864 | 3.606  | 1.000 | 22.24 |
| ATOM | 667 | ND2 | ASN | A | 107 | -6.328  | 23.567 | 5.634  | 1.000 | 26.27 |
| ATOM | 668 | C   | ASN | A | 107 | -9.273  | 20.581 | 5.877  | 1.000 | 38.65 |
| ATOM | 669 | O   | ASN | A | 107 | -10.274 | 20.887 | 5.236  | 1.000 | 46.02 |
| ATOM | 670 | N   | ASN | A | 108 | -9.002  | 19.431 | 6.465  | 1.000 | 30.37 |
| ATOM | 671 | CA  | ASN | A | 108 | -9.700  | 18.170 | 6.282  | 1.000 | 36.09 |
| ATOM | 672 | CB  | ASN | A | 108 | -8.676  | 17.017 | 6.195  | 1.000 | 40.88 |
| ATOM | 673 | CG  | ASN | A | 108 | -7.647  | 17.276 | 5.099  | 1.000 | 44.34 |
| ATOM | 674 | OD1 | ASN | A | 108 | -7.988  | 17.259 | 3.914  | 1.000 | 26.73 |
| ATOM | 675 | ND2 | ASN | A | 108 | -6.392  | 17.525 | 5.466  | 1.000 | 23.01 |

**FIGURE 214**

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|      |     |     |     |   |     |         |        |        |       |       |
|------|-----|-----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 676 | C   | ASN | A | 108 | -10.712 | 17.862 | 7.369  | 1.000 | 27.84 |
| ATOM | 677 | O   | ASN | A | 108 | -11.746 | 17.240 | 7.087  | 1.000 | 45.47 |
| ATOM | 678 | N   | PHE | A | 109 | -10.515 | 18.262 | 8.614  | 1.000 | 28.68 |
| ATOM | 679 | CA  | PHE | A | 109 | -11.601 | 17.986 | 9.569  | 1.000 | 29.14 |
| ATOM | 680 | CB  | PHE | A | 109 | -11.727 | 16.503 | 9.837  | 1.000 | 33.67 |
| ATOM | 681 | CG  | PHE | A | 109 | -10.501 | 15.678 | 10.128 | 1.000 | 32.21 |
| ATOM | 682 | CD1 | PHE | A | 109 | -9.720  | 15.199 | 9.088  | 1.000 | 36.73 |
| ATOM | 683 | CE1 | PHE | A | 109 | -8.604  | 14.419 | 9.325  | 1.000 | 33.86 |
| ATOM | 684 | CZ  | PHE | A | 109 | -8.275  | 14.120 | 10.633 | 1.000 | 42.76 |
| ATOM | 685 | CE2 | PHE | A | 109 | -9.036  | 14.590 | 11.683 | 1.000 | 37.98 |
| ATOM | 686 | CD2 | PHE | A | 109 | -10.143 | 15.376 | 11.430 | 1.000 | 37.01 |
| ATOM | 687 | C   | PHE | A | 109 | -11.450 | 18.785 | 10.856 | 1.000 | 28.59 |
| ATOM | 688 | O   | PHE | A | 109 | -10.493 | 19.529 | 11.101 | 1.000 | 25.57 |
| ATOM | 689 | N   | ARG | A | 110 | -12.457 | 18.692 | 11.728 | 1.000 | 29.57 |
| ATOM | 690 | CA  | ARG | A | 110 | -12.560 | 19.633 | 12.835 | 1.000 | 29.56 |
| ATOM | 691 | CB  | ARG | A | 110 | -13.912 | 19.447 | 13.560 | 1.000 | 39.08 |
| ATOM | 692 | CG  | ARG | A | 110 | -15.115 | 19.581 | 12.647 | 1.000 | 51.99 |
| ATOM | 693 | CD  | ARG | A | 110 | -15.714 | 20.978 | 12.671 | 1.000 | 60.61 |
| ATOM | 694 | NE  | ARG | A | 110 | -16.438 | 21.295 | 11.439 | 1.000 | 56.28 |
| ATOM | 695 | CZ  | ARG | A | 110 | -17.049 | 22.446 | 11.187 | 1.000 | 59.30 |
| ATOM | 696 | NH1 | ARG | A | 110 | -17.685 | 22.657 | 10.040 | 1.000 | 45.23 |
| ATOM | 697 | NH2 | ARG | A | 110 | -17.032 | 23.413 | 12.100 | 1.000 | 84.92 |
| ATOM | 698 | C   | ARG | A | 110 | -11.462 | 19.550 | 13.898 | 1.000 | 32.92 |
| ATOM | 699 | O   | ARG | A | 110 | -10.952 | 20.588 | 14.359 | 1.000 | 36.08 |
| ATOM | 700 | N   | ARG | A | 111 | -11.163 | 18.325 | 14.281 | 1.000 | 28.03 |
| ATOM | 701 | CA  | ARG | A | 111 | -10.152 | 17.978 | 15.275 | 1.000 | 26.59 |
| ATOM | 702 | CB  | ARG | A | 111 | -10.714 | 17.032 | 16.339 | 1.000 | 33.75 |
| ATOM | 703 | CG  | ARG | A | 111 | -11.497 | 17.792 | 17.422 | 1.000 | 39.79 |
| ATOM | 704 | CD  | ARG | A | 111 | -12.543 | 16.891 | 18.038 | 1.000 | 40.61 |
| ATOM | 705 | NE  | ARG | A | 111 | -13.133 | 17.383 | 19.283 | 1.000 | 34.63 |
| ATOM | 706 | CZ  | ARG | A | 111 | -13.380 | 16.499 | 20.268 | 1.000 | 44.09 |
| ATOM | 707 | NH1 | ARG | A | 111 | -13.087 | 15.209 | 20.117 | 1.000 | 40.26 |
| ATOM | 708 | NH2 | ARG | A | 111 | -13.915 | 16.924 | 21.402 | 1.000 | 48.99 |
| ATOM | 709 | C   | ARG | A | 111 | -8.977  | 17.326 | 14.564 | 1.000 | 26.23 |
| ATOM | 710 | O   | ARG | A | 111 | -8.583  | 16.195 | 14.813 | 1.000 | 22.76 |
| ATOM | 711 | N   | GLU | A | 112 | -8.437  | 18.086 | 13.603 | 1.000 | 18.42 |
| ATOM | 712 | CA  | GLU | A | 112 | -7.400  | 17.493 | 12.752 | 1.000 | 19.07 |
| ATOM | 713 | CB  | GLU | A | 112 | -7.339  | 18.364 | 11.470 | 1.000 | 13.71 |
| ATOM | 714 | CG  | GLU | A | 112 | -6.317  | 17.831 | 10.484 | 1.000 | 14.61 |
| ATOM | 715 | CD  | GLU | A | 112 | -6.654  | 18.208 | 9.049  | 1.000 | 20.17 |
| ATOM | 716 | OE1 | GLU | A | 112 | -7.701  | 18.836 | 8.814  | 1.000 | 23.80 |
| ATOM | 717 | OE2 | GLU | A | 112 | -5.819  | 17.872 | 8.184  | 1.000 | 20.53 |
| ATOM | 718 | C   | GLU | A | 112 | -6.059  | 17.425 | 13.457 | 1.000 | 13.05 |
| ATOM | 719 | O   | GLU | A | 112 | -5.177  | 16.583 | 13.179 | 1.000 | 16.04 |
| ATOM | 720 | N   | TYR | A | 113 | -5.888  | 18.365 | 14.392 | 1.000 | 14.44 |
| ATOM | 721 | CA  | TYR | A | 113 | -4.660  | 18.455 | 15.170 | 1.000 | 14.56 |
| ATOM | 722 | CB  | TYR | A | 113 | -3.783  | 19.667 | 14.843 | 1.000 | 13.32 |
| ATOM | 723 | CG  | TYR | A | 113 | -3.500  | 19.908 | 13.376 | 1.000 | 17.76 |
| ATOM | 724 | CD1 | TYR | A | 113 | -2.393  | 19.395 | 12.721 | 1.000 | 18.07 |
| ATOM | 725 | CE1 | TYR | A | 113 | -2.151  | 19.630 | 11.364 | 1.000 | 14.90 |
| ATOM | 726 | CZ  | TYR | A | 113 | -3.049  | 20.406 | 10.658 | 1.000 | 18.66 |
| ATOM | 727 | OH  | TYR | A | 113 | -2.860  | 20.666 | 9.306  | 1.000 | 17.72 |

**FIGURE 215**

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 728 | CE2 | TYR | A | 113 | -4.162 | 20.925 | 11.293 | 1.000 | 20.77 |
| ATOM | 729 | CD2 | TYR | A | 113 | -4.392 | 20.683 | 12.633 | 1.000 | 15.75 |
| ATOM | 730 | C   | TYR | A | 113 | -4.980 | 18.563 | 16.668 | 1.000 | 15.81 |
| ATOM | 731 | O   | TYR | A | 113 | -5.993 | 19.136 | 17.046 | 1.000 | 16.02 |
| ATOM | 732 | N   | ILE | A | 114 | -4.051 | 18.047 | 17.461 | 1.000 | 12.86 |
| ATOM | 733 | CA  | ILE | A | 114 | -4.004 | 18.364 | 18.882 | 1.000 | 12.93 |
| ATOM | 734 | CB  | ILE | A | 114 | -4.060 | 17.088 | 19.740 | 1.000 | 17.81 |
| ATOM | 735 | CG1 | ILE | A | 114 | -5.461 | 16.478 | 19.730 | 1.000 | 20.46 |
| ATOM | 736 | CD1 | ILE | A | 114 | -5.604 | 15.068 | 20.250 | 1.000 | 18.86 |
| ATOM | 737 | CG2 | ILE | A | 114 | -3.565 | 17.380 | 21.156 | 1.000 | 18.53 |
| ATOM | 738 | C   | ILE | A | 114 | -2.712 | 19.118 | 19.104 | 1.000 | 14.86 |
| ATOM | 739 | O   | ILE | A | 114 | -1.650 | 18.594 | 18.750 | 1.000 | 17.75 |
| ATOM | 740 | N   | VAL | A | 115 | -2.797 | 20.311 | 19.631 | 1.000 | 16.67 |
| ATOM | 741 | CA  | VAL | A | 115 | -1.600 | 21.072 | 19.972 | 1.000 | 13.98 |
| ATOM | 742 | CB  | VAL | A | 115 | -1.749 | 22.543 | 19.584 | 1.000 | 14.73 |
| ATOM | 743 | CG1 | VAL | A | 115 | -0.680 | 23.353 | 20.303 | 1.000 | 27.44 |
| ATOM | 744 | CG2 | VAL | A | 115 | -1.659 | 22.643 | 18.059 | 1.000 | 22.61 |
| ATOM | 745 | C   | VAL | A | 115 | -1.360 | 20.975 | 21.472 | 1.000 | 13.84 |
| ATOM | 746 | O   | VAL | A | 115 | -2.303 | 21.113 | 22.246 | 1.000 | 17.38 |
| ATOM | 747 | N   | THR | A | 116 | -0.116 | 20.748 | 21.863 | 1.000 | 13.55 |
| ATOM | 748 | CA  | THR | A | 116 | 0.108  | 20.593 | 23.304 | 1.000 | 17.85 |
| ATOM | 749 | CB  | THR | A | 116 | -0.042 | 19.101 | 23.682 | 1.000 | 16.90 |
| ATOM | 750 | OG1 | THR | A | 116 | -0.019 | 18.974 | 25.104 | 1.000 | 16.67 |
| ATOM | 751 | CG2 | THR | A | 116 | 1.092  | 18.252 | 23.118 | 1.000 | 18.44 |
| ATOM | 752 | C   | THR | A | 116 | 1.462  | 21.186 | 23.681 | 1.000 | 14.01 |
| ATOM | 753 | O   | THR | A | 116 | 2.258  | 21.452 | 22.775 | 1.000 | 13.95 |
| ATOM | 754 | N   | GLN | A | 117 | 1.702  | 21.380 | 24.961 | 1.000 | 15.16 |
| ATOM | 755 | CA  | GLN | A | 117 | 3.032  | 21.825 | 25.403 | 1.000 | 20.32 |
| ATOM | 756 | CB  | GLN | A | 117 | 2.866  | 22.383 | 26.829 | 1.000 | 17.18 |
| ATOM | 757 | CG  | GLN | A | 117 | 2.751  | 21.245 | 27.841 | 1.000 | 23.10 |
| ATOM | 758 | CD  | GLN | A | 117 | 2.459  | 21.700 | 29.254 | 1.000 | 22.85 |
| ATOM | 759 | OE1 | GLN | A | 117 | 2.255  | 22.879 | 29.560 | 1.000 | 19.09 |
| ATOM | 760 | NE2 | GLN | A | 117 | 2.428  | 20.740 | 30.181 | 1.000 | 25.28 |
| ATOM | 761 | C   | GLN | A | 117 | 4.051  | 20.714 | 25.344 | 1.000 | 22.35 |
| ATOM | 762 | O   | GLN | A | 117 | 3.743  | 19.524 | 25.186 | 1.000 | 21.90 |
| ATOM | 763 | N   | GLY | A | 118 | 5.348  | 20.995 | 25.467 | 1.000 | 20.42 |
| ATOM | 764 | CA  | GLY | A | 118 | 6.280  | 19.856 | 25.478 | 1.000 | 16.32 |
| ATOM | 765 | C   | GLY | A | 118 | 6.111  | 19.186 | 26.830 | 1.000 | 14.48 |
| ATOM | 766 | O   | GLY | A | 118 | 6.206  | 19.869 | 27.834 | 1.000 | 20.82 |
| ATOM | 767 | N   | PRO | A | 119 | 5.850  | 17.888 | 26.898 | 1.000 | 19.04 |
| ATOM | 768 | CA  | PRO | A | 119 | 5.598  | 17.210 | 28.158 | 1.000 | 17.15 |
| ATOM | 769 | CB  | PRO | A | 119 | 5.626  | 15.716 | 27.778 | 1.000 | 17.56 |
| ATOM | 770 | CG  | PRO | A | 119 | 5.109  | 15.747 | 26.360 | 1.000 | 16.78 |
| ATOM | 771 | CD  | PRO | A | 119 | 5.766  | 16.966 | 25.749 | 1.000 | 16.98 |
| ATOM | 772 | C   | PRO | A | 119 | 6.686  | 17.470 | 29.215 | 1.000 | 14.53 |
| ATOM | 773 | O   | PRO | A | 119 | 7.852  | 17.580 | 28.857 | 1.000 | 20.14 |
| ATOM | 774 | N   | LEU | A | 120 | 6.193  | 17.562 | 30.436 | 1.000 | 20.34 |
| ATOM | 775 | CA  | LEU | A | 120 | 7.014  | 17.632 | 31.639 | 1.000 | 26.17 |
| ATOM | 776 | CB  | LEU | A | 120 | 6.259  | 18.379 | 32.752 | 1.000 | 18.48 |
| ATOM | 777 | CG  | LEU | A | 120 | 6.077  | 19.879 | 32.495 | 1.000 | 23.01 |
| ATOM | 778 | CD1 | LEU | A | 120 | 4.937  | 20.427 | 33.332 | 1.000 | 23.31 |
| ATOM | 779 | CD2 | LEU | A | 120 | 7.399  | 20.586 | 32.764 | 1.000 | 24.84 |

**FIGURE 216**

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 780 | C   | LEU | A | 120 | 7.358  | 16.227 | 32.124 | 1.000 | 25.96 |
| ATOM | 781 | O   | LEU | A | 120 | 6.667  | 15.274 | 31.750 | 1.000 | 21.42 |
| ATOM | 782 | N   | PRO | A | 121 | 8.381  | 16.072 | 32.957 | 1.000 | 29.05 |
| ATOM | 783 | CA  | PRO | A | 121 | 8.595  | 14.786 | 33.629 | 1.000 | 25.75 |
| ATOM | 784 | CB  | PRO | A | 121 | 9.597  | 15.156 | 34.739 | 1.000 | 25.40 |
| ATOM | 785 | CG  | PRO | A | 121 | 10.409 | 16.244 | 34.108 | 1.000 | 27.02 |
| ATOM | 786 | CD  | PRO | A | 121 | 9.405  | 17.064 | 33.325 | 1.000 | 27.21 |
| ATOM | 787 | C   | PRO | A | 121 | 7.317  | 14.251 | 34.258 | 1.000 | 22.30 |
| ATOM | 788 | O   | PRO | A | 121 | 7.004  | 13.056 | 34.125 | 1.000 | 25.28 |
| ATOM | 789 | N   | GLY | A | 122 | 6.557  | 15.136 | 34.914 | 1.000 | 18.79 |
| ATOM | 790 | CA  | GLY | A | 122 | 5.347  | 14.719 | 35.583 | 1.000 | 16.68 |
| ATOM | 791 | C   | GLY | A | 122 | 4.075  | 14.740 | 34.751 | 1.000 | 28.03 |
| ATOM | 792 | O   | GLY | A | 122 | 3.020  | 14.526 | 35.376 | 1.000 | 24.04 |
| ATOM | 793 | N   | THR | A | 123 | 4.110  | 14.977 | 33.436 | 1.000 | 20.34 |
| ATOM | 794 | CA  | THR | A | 123 | 2.930  | 14.937 | 32.578 | 1.000 | 14.07 |
| ATOM | 795 | CB  | THR | A | 123 | 2.534  | 16.297 | 31.970 | 1.000 | 14.80 |
| ATOM | 796 | OG1 | THR | A | 123 | 3.597  | 16.765 | 31.130 | 1.000 | 20.06 |
| ATOM | 797 | CG2 | THR | A | 123 | 2.290  | 17.355 | 33.043 | 1.000 | 21.03 |
| ATOM | 798 | C   | THR | A | 123 | 3.121  | 13.982 | 31.401 | 1.000 | 17.25 |
| ATOM | 799 | O   | THR | A | 123 | 2.189  | 13.769 | 30.625 | 1.000 | 19.21 |
| ATOM | 800 | N   | LYS | A | 124 | 4.290  | 13.385 | 31.258 | 1.000 | 17.35 |
| ATOM | 801 | CA  | LYS | A | 124 | 4.591  | 12.474 | 30.157 | 1.000 | 20.84 |
| ATOM | 802 | CB  | LYS | A | 124 | 6.056  | 12.057 | 30.163 | 1.000 | 23.80 |
| ATOM | 803 | CG  | LYS | A | 124 | 6.574  | 11.185 | 31.268 | 1.000 | 22.00 |
| ATOM | 804 | CD  | LYS | A | 124 | 8.053  | 10.832 | 31.082 | 1.000 | 30.29 |
| ATOM | 805 | CE  | LYS | A | 124 | 8.441  | 9.720  | 32.044 | 1.000 | 45.34 |
| ATOM | 806 | NZ  | LYS | A | 124 | 9.868  | 9.696  | 32.452 | 1.000 | 41.63 |
| ATOM | 807 | C   | LYS | A | 124 | 3.636  | 11.275 | 30.163 | 1.000 | 19.38 |
| ATOM | 808 | O   | LYS | A | 124 | 3.239  | 10.855 | 29.071 | 1.000 | 19.48 |
| ATOM | 809 | N   | ASP | A | 125 | 3.233  | 10.748 | 31.314 | 1.000 | 20.33 |
| ATOM | 810 | CA  | ASP | A | 125 | 2.250  | 9.666  | 31.286 | 1.000 | 20.85 |
| ATOM | 811 | CB  | ASP | A | 125 | 2.042  | 9.048  | 32.667 | 1.000 | 21.24 |
| ATOM | 812 | CG  | ASP | A | 125 | 3.216  | 8.294  | 33.256 | 1.000 | 23.35 |
| ATOM | 813 | OD1 | ASP | A | 125 | 4.196  | 8.028  | 32.528 | 1.000 | 20.34 |
| ATOM | 814 | OD2 | ASP | A | 125 | 3.124  | 7.972  | 34.488 | 1.000 | 20.58 |
| ATOM | 815 | C   | ASP | A | 125 | 0.903  | 10.155 | 30.758 | 1.000 | 18.95 |
| ATOM | 816 | O   | ASP | A | 125 | 0.264  | 9.434  | 29.979 | 1.000 | 17.28 |
| ATOM | 817 | N   | ASP | A | 126 | 0.462  | 11.327 | 31.199 | 1.000 | 20.58 |
| ATOM | 818 | CA  | ASP | A | 126 | -0.740 | 11.974 | 30.672 | 1.000 | 16.25 |
| ATOM | 819 | CB  | ASP | A | 126 | -0.971 | 13.331 | 31.325 | 1.000 | 22.07 |
| ATOM | 820 | CG  | ASP | A | 126 | -1.198 | 13.393 | 32.813 | 1.000 | 35.20 |
| ATOM | 821 | OD1 | ASP | A | 126 | -1.760 | 12.424 | 33.363 | 1.000 | 28.11 |
| ATOM | 822 | OD2 | ASP | A | 126 | -0.833 | 14.421 | 33.448 | 1.000 | 29.77 |
| ATOM | 823 | C   | ASP | A | 126 | -0.636 | 12.184 | 29.153 | 1.000 | 14.70 |
| ATOM | 824 | O   | ASP | A | 126 | -1.589 | 11.970 | 28.403 | 1.000 | 17.56 |
| ATOM | 825 | N   | PHE | A | 127 | 0.509  | 12.629 | 28.658 | 1.000 | 16.52 |
| ATOM | 826 | CA  | PHE | A | 127 | 0.641  | 12.855 | 27.203 | 1.000 | 16.00 |
| ATOM | 827 | CB  | PHE | A | 127 | 2.039  | 13.358 | 26.853 | 1.000 | 16.31 |
| ATOM | 828 | CG  | PHE | A | 127 | 2.432  | 13.364 | 25.376 | 1.000 | 15.99 |
| ATOM | 829 | CD1 | PHE | A | 127 | 2.178  | 14.498 | 24.615 | 1.000 | 18.51 |
| ATOM | 830 | CE1 | PHE | A | 127 | 2.518  | 14.549 | 23.273 | 1.000 | 10.71 |
| ATOM | 831 | CZ  | PHE | A | 127 | 3.108  | 13.449 | 22.681 | 1.000 | 15.27 |

FIGURE 217

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 832 | CE2 | PHE | A | 127 | 3.382  | 12.289 | 23.403 | 1.000 | 19.04 |
| ATOM | 833 | CD2 | PHE | A | 127 | 3.061  | 12.299 | 24.747 | 1.000 | 16.38 |
| ATOM | 834 | C   | PHE | A | 127 | 0.385  | 11.547 | 26.468 | 1.000 | 22.45 |
| ATOM | 835 | O   | PHE | A | 127 | -0.332 | 11.482 | 25.478 | 1.000 | 16.59 |
| ATOM | 836 | N   | TRP | A | 128 | 1.052  | 10.479 | 26.939 | 1.000 | 15.18 |
| ATOM | 837 | CA  | TRP | A | 128 | 0.896  | 9.221  | 26.182 | 1.000 | 16.47 |
| ATOM | 838 | CB  | TRP | A | 128 | 1.938  | 8.201  | 26.653 | 1.000 | 14.81 |
| ATOM | 839 | CG  | TRP | A | 128 | 3.329  | 8.492  | 26.170 | 1.000 | 17.83 |
| ATOM | 840 | CD1 | TRP | A | 128 | 4.444  | 8.788  | 26.892 | 1.000 | 15.04 |
| ATOM | 841 | NE1 | TRP | A | 128 | 5.526  | 8.987  | 26.043 | 1.000 | 16.38 |
| ATOM | 842 | CE2 | TRP | A | 128 | 5.110  | 8.818  | 24.749 | 1.000 | 15.72 |
| ATOM | 843 | CD2 | TRP | A | 128 | 3.738  | 8.509  | 24.787 | 1.000 | 15.19 |
| ATOM | 844 | CE3 | TRP | A | 128 | 3.062  | 8.282  | 23.587 | 1.000 | 16.34 |
| ATOM | 845 | CZ3 | TRP | A | 128 | 3.760  | 8.373  | 22.395 | 1.000 | 18.84 |
| ATOM | 846 | CH2 | TRP | A | 128 | 5.126  | 8.684  | 22.375 | 1.000 | 18.88 |
| ATOM | 847 | CZ2 | TRP | A | 128 | 5.797  | 8.906  | 23.544 | 1.000 | 19.59 |
| ATOM | 848 | C   | TRP | A | 128 | -0.516 | 8.680  | 26.335 | 1.000 | 18.33 |
| ATOM | 849 | O   | TRP | A | 128 | -1.095 | 8.039  | 25.441 | 1.000 | 17.84 |
| ATOM | 850 | N   | LYS | A | 129 | -1.136 | 8.925  | 27.490 | 1.000 | 16.01 |
| ATOM | 851 | CA  | LYS | A | 129 | -2.552 | 8.577  | 27.669 | 1.000 | 15.83 |
| ATOM | 852 | CB  | LYS | A | 129 | -2.959 | 8.905  | 29.107 | 1.000 | 16.11 |
| ATOM | 853 | CG  | LYS | A | 129 | -4.428 | 8.639  | 29.383 | 1.000 | 22.20 |
| ATOM | 854 | CD  | LYS | A | 129 | -4.734 | 8.820  | 30.866 | 1.000 | 21.45 |
| ATOM | 855 | CE  | LYS | A | 129 | -6.258 | 8.852  | 31.065 | 1.000 | 26.32 |
| ATOM | 856 | NZ  | LYS | A | 129 | -6.584 | 9.011  | 32.510 | 1.000 | 34.60 |
| ATOM | 857 | C   | LYS | A | 129 | -3.418 | 9.305  | 26.655 | 1.000 | 22.77 |
| ATOM | 858 | O   | LYS | A | 129 | -4.278 | 8.695  | 26.000 | 1.000 | 18.99 |
| ATOM | 859 | N   | MET | A | 130 | -3.188 | 10.621 | 26.479 | 1.000 | 15.75 |
| ATOM | 860 | CA  | MET | A | 130 | -3.893 | 11.366 | 25.434 | 1.000 | 13.41 |
| ATOM | 861 | CB  | MET | A | 130 | -3.416 | 12.840 | 25.476 | 1.000 | 16.79 |
| ATOM | 862 | CG  | MET | A | 130 | -4.077 | 13.682 | 24.379 | 1.000 | 18.60 |
| ATOM | 863 | SD  | MET | A | 130 | -3.548 | 15.406 | 24.457 | 1.000 | 18.90 |
| ATOM | 864 | CE  | MET | A | 130 | -1.867 | 15.262 | 23.906 | 1.000 | 14.57 |
| ATOM | 865 | C   | MET | A | 130 | -3.662 | 10.816 | 24.035 | 1.000 | 16.03 |
| ATOM | 866 | O   | MET | A | 130 | -4.577 | 10.636 | 23.228 | 1.000 | 21.60 |
| ATOM | 867 | N   | VAL | A | 131 | -2.421 | 10.513 | 23.688 | 1.000 | 16.52 |
| ATOM | 868 | CA  | VAL | A | 131 | -2.096 | 9.907  | 22.395 | 1.000 | 17.62 |
| ATOM | 869 | CB  | VAL | A | 131 | -0.576 | 9.659  | 22.293 | 1.000 | 15.16 |
| ATOM | 870 | CG1 | VAL | A | 131 | -0.228 | 8.757  | 21.118 | 1.000 | 16.01 |
| ATOM | 871 | CG2 | VAL | A | 131 | 0.162  | 10.996 | 22.200 | 1.000 | 14.77 |
| ATOM | 872 | C   | VAL | A | 131 | -2.891 | 8.614  | 22.198 | 1.000 | 14.71 |
| ATOM | 873 | O   | VAL | A | 131 | -3.480 | 8.392  | 21.126 | 1.000 | 17.34 |
| ATOM | 874 | N   | TRP | A | 132 | -2.952 | 7.787  | 23.223 | 1.000 | 14.88 |
| ATOM | 875 | CA  | TRP | A | 132 | -3.697 | 6.516  | 23.124 | 1.000 | 22.11 |
| ATOM | 876 | CB  | TRP | A | 132 | -3.433 | 5.620  | 24.339 | 1.000 | 22.48 |
| ATOM | 877 | CG  | TRP | A | 132 | -4.168 | 4.301  | 24.280 | 1.000 | 27.32 |
| ATOM | 878 | CD1 | TRP | A | 132 | -5.262 | 3.909  | 25.019 | 1.000 | 25.14 |
| ATOM | 879 | NE1 | TRP | A | 132 | -5.611 | 2.623  | 24.645 | 1.000 | 23.87 |
| ATOM | 880 | CE2 | TRP | A | 132 | -4.763 | 2.172  | 23.681 | 1.000 | 18.18 |
| ATOM | 881 | CD2 | TRP | A | 132 | -3.834 | 3.198  | 23.418 | 1.000 | 18.05 |
| ATOM | 882 | CE3 | TRP | A | 132 | -2.840 | 2.999  | 22.460 | 1.000 | 22.17 |
| ATOM | 883 | CZ3 | TRP | A | 132 | -2.774 | 1.795  | 21.772 | 1.000 | 28.54 |

**FIGURE 218**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 884 | CH2 | TRP | A | 132 | -3.721 | 0.806  | 22.066 | 1.000 | 23.87 |
| ATOM | 885 | CZ2 | TRP | A | 132 | -4.696 | 0.966  | 22.993 | 1.000 | 20.35 |
| ATOM | 886 | C   | TRP | A | 132 | -5.193 | 6.750  | 22.947 | 1.000 | 17.05 |
| ATOM | 887 | O   | TRP | A | 132 | -5.818 | 6.256  | 21.987 | 1.000 | 20.64 |
| ATOM | 888 | N   | GLU | A | 133 | -5.791 | 7.519  | 23.839 | 1.000 | 14.90 |
| ATOM | 889 | CA  | GLU | A | 133 | -7.219 | 7.778  | 23.820 | 1.000 | 17.45 |
| ATOM | 890 | CB  | GLU | A | 133 | -7.610 | 8.589  | 25.078 | 1.000 | 18.05 |
| ATOM | 891 | CG  | GLU | A | 133 | -7.397 | 7.760  | 26.341 | 1.000 | 19.08 |
| ATOM | 892 | CD  | GLU | A | 133 | -7.868 | 8.505  | 27.588 | 1.000 | 27.21 |
| ATOM | 893 | OE1 | GLU | A | 133 | -8.176 | 9.707  | 27.515 | 1.000 | 24.17 |
| ATOM | 894 | OE2 | GLU | A | 133 | -7.926 | 7.874  | 28.661 | 1.000 | 32.77 |
| ATOM | 895 | C   | GLU | A | 133 | -7.680 | 8.510  | 22.579 | 1.000 | 20.80 |
| ATOM | 896 | O   | GLU | A | 133 | -8.825 | 8.300  | 22.156 | 1.000 | 22.88 |
| ATOM | 897 | N   | GLN | A | 134 | -6.829 | 9.358  | 22.026 | 1.000 | 17.73 |
| ATOM | 898 | CA  | GLN | A | 134 | -7.237 | 10.221 | 20.900 | 1.000 | 16.57 |
| ATOM | 899 | CB  | GLN | A | 134 | -6.549 | 11.579 | 21.008 | 1.000 | 14.29 |
| ATOM | 900 | CG  | GLN | A | 134 | -6.990 | 12.288 | 22.299 | 1.000 | 16.77 |
| ATOM | 901 | CD  | GLN | A | 134 | -8.452 | 12.650 | 22.274 | 1.000 | 21.52 |
| ATOM | 902 | OE1 | GLN | A | 134 | -9.006 | 13.127 | 21.277 | 1.000 | 27.29 |
| ATOM | 903 | NE2 | GLN | A | 134 | -9.111 | 12.430 | 23.414 | 1.000 | 22.22 |
| ATOM | 904 | C   | GLN | A | 134 | -6.950 | 9.599  | 19.542 | 1.000 | 19.42 |
| ATOM | 905 | O   | GLN | A | 134 | -7.196 | 10.269 | 18.542 | 1.000 | 18.38 |
| ATOM | 906 | N   | ASN | A | 135 | -6.467 | 8.362  | 19.537 | 1.000 | 19.05 |
| ATOM | 907 | CA  | ASN | A | 135 | -6.213 | 7.579  | 18.343 | 1.000 | 19.16 |
| ATOM | 908 | CB  | ASN | A | 135 | -7.480 | 7.376  | 17.494 | 1.000 | 20.31 |
| ATOM | 909 | CG  | ASN | A | 135 | -8.541 | 6.596  | 18.257 | 1.000 | 31.86 |
| ATOM | 910 | OD1 | ASN | A | 135 | -8.283 | 5.493  | 18.725 | 1.000 | 33.23 |
| ATOM | 911 | ND2 | ASN | A | 135 | -9.742 | 7.149  | 18.391 | 1.000 | 30.19 |
| ATOM | 912 | C   | ASN | A | 135 | -5.155 | 8.263  | 17.482 | 1.000 | 17.39 |
| ATOM | 913 | O   | ASN | A | 135 | -5.206 | 8.264  | 16.256 | 1.000 | 22.39 |
| ATOM | 914 | N   | VAL | A | 136 | -4.196 | 8.866  | 18.167 | 1.000 | 14.13 |
| ATOM | 915 | CA  | VAL | A | 136 | -3.123 | 9.563  | 17.457 | 1.000 | 16.02 |
| ATOM | 916 | CB  | VAL | A | 136 | -2.417 | 10.541 | 18.433 | 1.000 | 18.99 |
| ATOM | 917 | CG1 | VAL | A | 136 | -1.100 | 11.000 | 17.793 | 1.000 | 20.47 |
| ATOM | 918 | CG2 | VAL | A | 136 | -3.330 | 11.692 | 18.794 | 1.000 | 13.05 |
| ATOM | 919 | C   | VAL | A | 136 | -2.120 | 8.585  | 16.871 | 1.000 | 18.76 |
| ATOM | 920 | O   | VAL | A | 136 | -1.653 | 7.669  | 17.563 | 1.000 | 17.38 |
| ATOM | 921 | N   | HIS | A | 137 | -1.756 | 8.745  | 15.591 | 1.000 | 15.53 |
| ATOM | 922 | CA  | HIS | A | 137 | -0.715 | 7.888  | 15.035 | 1.000 | 18.61 |
| ATOM | 923 | CB  | HIS | A | 137 | -1.197 | 7.109  | 13.799 | 1.000 | 19.72 |
| ATOM | 924 | CG  | HIS | A | 137 | -2.274 | 6.119  | 14.090 | 1.000 | 22.80 |
| ATOM | 925 | ND1 | HIS | A | 137 | -3.478 | 6.436  | 14.669 | 1.000 | 26.95 |
| ATOM | 926 | CE1 | HIS | A | 137 | -4.209 | 5.343  | 14.795 | 1.000 | 30.61 |
| ATOM | 927 | NE2 | HIS | A | 137 | -3.516 | 4.331  | 14.319 | 1.000 | 27.83 |
| ATOM | 928 | CD2 | HIS | A | 137 | -2.301 | 4.778  | 13.869 | 1.000 | 31.20 |
| ATOM | 929 | C   | HIS | A | 137 | 0.523  | 8.677  | 14.620 | 1.000 | 19.42 |
| ATOM | 930 | O   | HIS | A | 137 | 1.534  | 8.071  | 14.287 | 1.000 | 19.32 |
| ATOM | 931 | N   | ASN | A | 138 | 0.469  | 10.009 | 14.624 | 1.000 | 18.64 |
| ATOM | 932 | CA  | ASN | A | 138 | 1.609  | 10.809 | 14.197 | 1.000 | 16.59 |
| ATOM | 933 | CB  | ASN | A | 138 | 1.368  | 11.460 | 12.823 | 1.000 | 14.79 |
| ATOM | 934 | CG  | ASN | A | 138 | 1.182  | 10.388 | 11.774 | 1.000 | 14.32 |
| ATOM | 935 | OD1 | ASN | A | 138 | 0.070  | 10.154 | 11.277 | 1.000 | 23.35 |

**FIGURE 219**

|      |     |     |     |   |     |        |        |        |       |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 936 | ND2 | ASN | A | 138 | 2.272  | 9.719  | 11.442 | 1.000 | 15.72 |
| ATOM | 937 | C   | ASN | A | 138 | 1.882  | 11.894 | 15.224 | 1.000 | 17.49 |
| ATOM | 938 | O   | ASN | A | 138 | 0.923  | 12.540 | 15.639 | 1.000 | 16.64 |
| ATOM | 939 | N   | ILE | A | 139 | 3.138  | 12.081 | 15.595 | 1.000 | 13.57 |
| ATOM | 940 | CA  | ILE | A | 139 | 3.492  | 13.222 | 16.443 | 1.000 | 13.49 |
| ATOM | 941 | CB  | ILE | A | 139 | 4.046  | 12.705 | 17.788 | 1.000 | 15.96 |
| ATOM | 942 | CG1 | ILE | A | 139 | 3.032  | 11.892 | 18.597 | 1.000 | 17.56 |
| ATOM | 943 | CD1 | ILE | A | 139 | 3.647  | 11.054 | 19.710 | 1.000 | 16.60 |
| ATOM | 944 | CG2 | ILE | A | 139 | 4.641  | 13.849 | 18.601 | 1.000 | 17.93 |
| ATOM | 945 | C   | ILE | A | 139 | 4.545  | 14.100 | 15.776 | 1.000 | 16.72 |
| ATOM | 946 | O   | ILE | A | 139 | 5.507  | 13.555 | 15.211 | 1.000 | 18.97 |
| ATOM | 947 | N   | VAL | A | 140 | 4.378  | 15.416 | 15.843 | 1.000 | 15.29 |
| ATOM | 948 | CA  | VAL | A | 140 | 5.330  | 16.361 | 15.282 | 1.000 | 15.83 |
| ATOM | 949 | CB  | VAL | A | 140 | 4.672  | 17.254 | 14.202 | 1.000 | 17.91 |
| ATOM | 950 | CG1 | VAL | A | 140 | 5.691  | 18.249 | 13.647 | 1.000 | 18.30 |
| ATOM | 951 | CG2 | VAL | A | 140 | 4.073  | 16.418 | 13.086 | 1.000 | 14.97 |
| ATOM | 952 | C   | VAL | A | 140 | 5.892  | 17.200 | 16.427 | 1.000 | 15.79 |
| ATOM | 953 | O   | VAL | A | 140 | 5.144  | 17.816 | 17.200 | 1.000 | 16.44 |
| ATOM | 954 | N   | MET | A | 141 | 7.208  | 17.203 | 16.579 | 1.000 | 16.25 |
| ATOM | 955 | CA  | MET | A | 141 | 7.900  | 17.899 | 17.660 | 1.000 | 21.24 |
| ATOM | 956 | CB  | MET | A | 141 | 8.745  | 16.916 | 18.480 | 1.000 | 18.76 |
| ATOM | 957 | CG  | MET | A | 141 | 9.555  | 17.528 | 19.619 | 1.000 | 15.74 |
| ATOM | 958 | SD  | MET | A | 141 | 10.162 | 16.187 | 20.709 | 1.000 | 19.42 |
| ATOM | 959 | CE  | MET | A | 141 | 11.299 | 17.174 | 21.703 | 1.000 | 22.74 |
| ATOM | 960 | C   | MET | A | 141 | 8.795  | 18.989 | 17.072 | 1.000 | 14.50 |
| ATOM | 961 | O   | MET | A | 141 | 9.715  | 18.659 | 16.332 | 1.000 | 19.95 |
| ATOM | 962 | N   | VAL | A | 142 | 8.551  | 20.246 | 17.347 | 1.000 | 18.34 |
| ATOM | 963 | CA  | VAL | A | 142 | 9.296  | 21.313 | 16.698 | 1.000 | 19.48 |
| ATOM | 964 | CB  | VAL | A | 142 | 8.396  | 22.310 | 15.933 | 1.000 | 22.88 |
| ATOM | 965 | CG1 | VAL | A | 142 | 9.226  | 22.965 | 14.836 | 1.000 | 28.48 |
| ATOM | 966 | CG2 | VAL | A | 142 | 7.180  | 21.668 | 15.294 | 1.000 | 30.53 |
| ATOM | 967 | C   | VAL | A | 142 | 10.112 | 22.075 | 17.732 | 1.000 | 23.04 |
| ATOM | 968 | O   | VAL | A | 142 | 9.990  | 23.280 | 17.923 | 1.000 | 23.56 |
| ATOM | 969 | N   | THR | A | 143 | 10.952 | 21.298 | 18.417 | 1.000 | 29.09 |
| ATOM | 970 | CA  | THR | A | 143 | 11.788 | 21.805 | 19.501 | 1.000 | 28.45 |
| ATOM | 971 | CB  | THR | A | 143 | 10.984 | 22.204 | 20.751 | 1.000 | 26.09 |
| ATOM | 972 | OG1 | THR | A | 143 | 11.837 | 22.963 | 21.620 | 1.000 | 30.17 |
| ATOM | 973 | CG2 | THR | A | 143 | 10.487 | 21.021 | 21.586 | 1.000 | 17.97 |
| ATOM | 974 | C   | THR | A | 143 | 12.829 | 20.744 | 19.826 | 1.000 | 29.90 |
| ATOM | 975 | O   | THR | A | 143 | 12.598 | 19.553 | 19.664 | 1.000 | 23.69 |
| ATOM | 976 | N   | GLN | A | 144 | 14.008 | 21.163 | 20.257 | 1.000 | 35.84 |
| ATOM | 977 | CA  | GLN | A | 144 | 14.993 | 20.221 | 20.781 | 1.000 | 28.60 |
| ATOM | 978 | CB  | GLN | A | 144 | 16.415 | 20.692 | 20.494 | 1.000 | 27.98 |
| ATOM | 979 | CG  | GLN | A | 144 | 16.871 | 20.426 | 19.061 | 1.000 | 31.33 |
| ATOM | 980 | CD  | GLN | A | 144 | 18.293 | 20.929 | 18.844 | 1.000 | 44.78 |
| ATOM | 981 | OE1 | GLN | A | 144 | 19.270 | 20.199 | 19.004 | 1.000 | 50.77 |
| ATOM | 982 | NE2 | GLN | A | 144 | 18.424 | 22.197 | 18.474 | 1.000 | 34.02 |
| ATOM | 983 | C   | GLN | A | 144 | 14.724 | 20.124 | 22.271 | 1.000 | 28.09 |
| ATOM | 984 | O   | GLN | A | 144 | 14.141 | 21.024 | 22.878 | 1.000 | 24.45 |
| ATOM | 985 | N   | CYS | A | 145 | 15.115 | 19.032 | 22.927 | 1.000 | 30.90 |
| ATOM | 986 | CA  | CYS | A | 145 | 14.856 | 18.998 | 24.365 | 1.000 | 21.87 |
| ATOM | 987 | CB  | CYS | A | 145 | 15.313 | 17.631 | 24.897 | 1.000 | 20.92 |

**FIGURE 220**



|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 988  | SG  | CYS | A | 145 | 14.184 | 16.278 | 24.463 | 1.000 | 30.08 |
| ATOM | 989  | C   | CYS | A | 145 | 15.601 | 20.109 | 25.083 | 1.000 | 26.27 |
| ATOM | 990  | O   | CYS | A | 145 | 15.152 | 20.691 | 26.056 | 1.000 | 25.34 |
| ATOM | 991  | N   | VAL | A | 146 | 16.795 | 20.375 | 24.555 | 1.000 | 27.66 |
| ATOM | 992  | CA  | VAL | A | 146 | 17.696 | 21.367 | 25.097 | 1.000 | 30.29 |
| ATOM | 993  | CB  | VAL | A | 146 | 18.963 | 20.721 | 25.711 | 1.000 | 36.55 |
| ATOM | 994  | CG1 | VAL | A | 146 | 19.918 | 21.827 | 26.139 | 1.000 | 34.60 |
| ATOM | 995  | CG2 | VAL | A | 146 | 18.601 | 19.795 | 26.859 | 1.000 | 44.23 |
| ATOM | 996  | C   | VAL | A | 146 | 18.213 | 22.307 | 24.014 | 1.000 | 28.45 |
| ATOM | 997  | O   | VAL | A | 146 | 18.841 | 21.790 | 23.076 | 1.000 | 40.86 |
| ATOM | 998  | N   | GLU | A | 147 | 17.971 | 23.586 | 24.167 | 1.000 | 28.57 |
| ATOM | 999  | CA  | GLU | A | 147 | 18.452 | 24.625 | 23.258 | 1.000 | 37.00 |
| ATOM | 1000 | CB  | GLU | A | 147 | 17.283 | 25.228 | 22.467 | 1.000 | 37.35 |
| ATOM | 1001 | CG  | GLU | A | 147 | 16.357 | 24.218 | 21.821 | 1.000 | 32.42 |
| ATOM | 1002 | CD  | GLU | A | 147 | 15.173 | 24.836 | 21.097 | 1.000 | 36.64 |
| ATOM | 1003 | OE1 | GLU | A | 147 | 14.684 | 25.926 | 21.465 | 1.000 | 28.99 |
| ATOM | 1004 | OE2 | GLU | A | 147 | 14.708 | 24.197 | 20.129 | 1.000 | 29.46 |
| ATOM | 1005 | C   | GLU | A | 147 | 19.191 | 25.727 | 24.028 | 1.000 | 41.02 |
| ATOM | 1006 | O   | GLU | A | 147 | 18.682 | 26.143 | 25.080 | 1.000 | 35.27 |
| ATOM | 1007 | N   | LYS | A | 148 | 20.338 | 26.211 | 23.559 | 1.000 | 49.35 |
| ATOM | 1008 | CA  | LYS | A | 148 | 21.141 | 27.170 | 24.317 | 1.000 | 50.64 |
| ATOM | 1009 | CB  | LYS | A | 148 | 20.525 | 28.547 | 24.520 | 1.000 | 54.31 |
| ATOM | 1010 | CG  | LYS | A | 148 | 21.448 | 29.714 | 24.766 | 1.000 | 56.11 |
| ATOM | 1011 | CD  | LYS | A | 148 | 22.091 | 29.906 | 26.107 | 1.000 | 51.55 |
| ATOM | 1012 | CE  | LYS | A | 148 | 23.607 | 30.019 | 26.124 | 1.000 | 45.10 |
| ATOM | 1013 | NZ  | LYS | A | 148 | 24.142 | 30.959 | 27.163 | 1.000 | 37.78 |
| ATOM | 1014 | C   | LYS | A | 148 | 21.369 | 26.580 | 25.712 | 1.000 | 33.28 |
| ATOM | 1015 | O   | LYS | A | 148 | 21.186 | 27.326 | 26.676 | 1.000 | 40.06 |
| ATOM | 1016 | N   | GLY | A | 149 | 21.686 | 25.282 | 25.751 | 1.000 | 23.87 |
| ATOM | 1017 | CA  | GLY | A | 149 | 21.915 | 24.686 | 27.061 | 1.000 | 33.16 |
| ATOM | 1018 | C   | GLY | A | 149 | 20.778 | 24.925 | 28.034 | 1.000 | 34.12 |
| ATOM | 1019 | O   | GLY | A | 149 | 20.966 | 24.992 | 29.241 | 1.000 | 33.20 |
| ATOM | 1020 | N   | ARG | A | 150 | 19.544 | 25.082 | 27.560 | 1.000 | 43.51 |
| ATOM | 1021 | CA  | ARG | A | 150 | 18.420 | 25.138 | 28.502 | 1.000 | 47.78 |
| ATOM | 1022 | CB  | ARG | A | 150 | 17.913 | 26.553 | 28.703 | 1.000 | 56.08 |
| ATOM | 1023 | CG  | ARG | A | 150 | 16.416 | 26.706 | 28.896 | 1.000 | 63.73 |
| ATOM | 1024 | CD  | ARG | A | 150 | 16.066 | 28.176 | 29.132 | 1.000 | 69.11 |
| ATOM | 1025 | NE  | ARG | A | 150 | 16.737 | 28.703 | 30.311 | 1.000 | 74.23 |
| ATOM | 1026 | CZ  | ARG | A | 150 | 16.496 | 29.840 | 30.951 | 1.000 | 82.40 |
| ATOM | 1027 | NH1 | ARG | A | 150 | 15.544 | 30.672 | 30.553 | 1.000 | 94.75 |
| ATOM | 1028 | NH2 | ARG | A | 150 | 17.228 | 30.148 | 32.023 | 1.000 | 84.24 |
| ATOM | 1029 | C   | ARG | A | 150 | 17.319 | 24.195 | 28.020 | 1.000 | 40.29 |
| ATOM | 1030 | O   | ARG | A | 150 | 17.214 | 23.897 | 26.826 | 1.000 | 44.43 |
| ATOM | 1031 | N   | VAL | A | 151 | 16.553 | 23.714 | 28.991 | 1.000 | 42.19 |
| ATOM | 1032 | CA  | VAL | A | 151 | 15.612 | 22.624 | 28.731 | 1.000 | 40.59 |
| ATOM | 1033 | CB  | VAL | A | 151 | 15.397 | 21.764 | 29.991 | 1.000 | 39.25 |
| ATOM | 1034 | CG1 | VAL | A | 151 | 16.743 | 21.494 | 30.643 | 1.000 | 35.31 |
| ATOM | 1035 | CG2 | VAL | A | 151 | 14.448 | 22.442 | 30.961 | 1.000 | 47.15 |
| ATOM | 1036 | C   | VAL | A | 151 | 14.286 | 23.143 | 28.204 | 1.000 | 34.87 |
| ATOM | 1037 | O   | VAL | A | 151 | 13.588 | 23.974 | 28.783 | 1.000 | 42.34 |
| ATOM | 1038 | N   | LYS | A | 152 | 13.921 | 22.633 | 27.028 | 1.000 | 34.21 |
| ATOM | 1039 | CA  | LYS | A | 152 | 12.658 | 23.089 | 26.435 | 1.000 | 32.45 |

FIGURE 221

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1040 | CB  | LYS | A | 152 | 12.936 | 23.469 | 24.983 | 1.000 | 29.05 |
| ATOM | 1041 | CG  | LYS | A | 152 | 13.723 | 24.774 | 24.884 | 1.000 | 40.50 |
| ATOM | 1042 | CD  | LYS | A | 152 | 13.161 | 25.824 | 25.832 | 1.000 | 34.61 |
| ATOM | 1043 | CE  | LYS | A | 152 | 12.890 | 27.143 | 25.135 | 1.000 | 41.44 |
| ATOM | 1044 | NZ  | LYS | A | 152 | 12.672 | 28.247 | 26.118 | 1.000 | 47.72 |
| ATOM | 1045 | C   | LYS | A | 152 | 11.580 | 22.023 | 26.534 | 1.000 | 32.08 |
| ATOM | 1046 | O   | LYS | A | 152 | 10.386 | 22.284 | 26.459 | 1.000 | 26.51 |
| ATOM | 1047 | N   | CYS | A | 153 | 11.986 | 20.771 | 26.708 | 1.000 | 26.76 |
| ATOM | 1048 | CA  | CYS | A | 153 | 11.021 | 19.668 | 26.654 | 1.000 | 25.46 |
| ATOM | 1049 | CB  | CYS | A | 153 | 10.682 | 19.380 | 25.189 | 1.000 | 21.77 |
| ATOM | 1050 | SG  | CYS | A | 153 | 9.398  | 18.138 | 24.927 | 1.000 | 22.14 |
| ATOM | 1051 | C   | CYS | A | 153 | 11.618 | 18.432 | 27.306 | 1.000 | 26.32 |
| ATOM | 1052 | O   | CYS | A | 153 | 12.824 | 18.201 | 27.158 | 1.000 | 25.23 |
| ATOM | 1053 | N   | ASP | A | 154 | 10.807 | 17.640 | 27.999 | 1.000 | 23.11 |
| ATOM | 1054 | CA  | ASP | A | 154 | 11.355 | 16.378 | 28.515 | 1.000 | 21.66 |
| ATOM | 1055 | CB  | ASP | A | 154 | 10.361 | 15.731 | 29.473 | 1.000 | 21.13 |
| ATOM | 1056 | CG  | ASP | A | 154 | 10.962 | 14.589 | 30.267 | 1.000 | 28.12 |
| ATOM | 1057 | OD1 | ASP | A | 154 | 11.961 | 14.786 | 30.981 | 1.000 | 33.22 |
| ATOM | 1058 | OD2 | ASP | A | 154 | 10.428 | 13.470 | 30.165 | 1.000 | 29.23 |
| ATOM | 1059 | C   | ASP | A | 154 | 11.654 | 15.413 | 27.380 | 1.000 | 25.41 |
| ATOM | 1060 | O   | ASP | A | 154 | 10.996 | 15.507 | 26.341 | 1.000 | 20.63 |
| ATOM | 1061 | N   | HIS | A | 155 | 12.599 | 14.484 | 27.555 | 1.000 | 22.40 |
| ATOM | 1062 | CA  | HIS | A | 155 | 12.785 | 13.364 | 26.630 | 1.000 | 23.74 |
| ATOM | 1063 | CB  | HIS | A | 155 | 14.212 | 12.842 | 26.726 | 1.000 | 20.26 |
| ATOM | 1064 | CG  | HIS | A | 155 | 14.625 | 11.929 | 25.619 | 1.000 | 22.14 |
| ATOM | 1065 | ND1 | HIS | A | 155 | 14.138 | 10.655 | 25.468 | 1.000 | 22.08 |
| ATOM | 1066 | CE1 | HIS | A | 155 | 14.671 | 10.085 | 24.412 | 1.000 | 22.58 |
| ATOM | 1067 | NE2 | HIS | A | 155 | 15.510 | 10.940 | 23.845 | 1.000 | 19.53 |
| ATOM | 1068 | CD2 | HIS | A | 155 | 15.484 | 12.098 | 24.594 | 1.000 | 24.73 |
| ATOM | 1069 | C   | HIS | A | 155 | 11.740 | 12.307 | 26.966 | 1.000 | 21.85 |
| ATOM | 1070 | O   | HIS | A | 155 | 11.993 | 11.292 | 27.629 | 1.000 | 26.15 |
| ATOM | 1071 | N   | TYR | A | 156 | 10.500 | 12.546 | 26.561 | 1.000 | 21.24 |
| ATOM | 1072 | CA  | TYR | A | 156 | 9.346  | 11.821 | 27.075 | 1.000 | 18.68 |
| ATOM | 1073 | CB  | TYR | A | 156 | 8.041  | 12.643 | 26.958 | 1.000 | 17.87 |
| ATOM | 1074 | CG  | TYR | A | 156 | 7.765  | 13.067 | 25.525 | 1.000 | 18.81 |
| ATOM | 1075 | CD1 | TYR | A | 156 | 7.032  | 12.280 | 24.647 | 1.000 | 23.10 |
| ATOM | 1076 | CE1 | TYR | A | 156 | 6.778  | 12.662 | 23.333 | 1.000 | 19.51 |
| ATOM | 1077 | CZ  | TYR | A | 156 | 7.267  | 13.880 | 22.886 | 1.000 | 17.53 |
| ATOM | 1078 | OH  | TYR | A | 156 | 7.003  | 14.236 | 21.579 | 1.000 | 16.54 |
| ATOM | 1079 | CE2 | TYR | A | 156 | 7.997  | 14.689 | 23.725 | 1.000 | 17.15 |
| ATOM | 1080 | CD2 | TYR | A | 156 | 8.247  | 14.285 | 25.047 | 1.000 | 15.43 |
| ATOM | 1081 | C   | TYR | A | 156 | 9.152  | 10.478 | 26.379 | 1.000 | 17.16 |
| ATOM | 1082 | O   | TYR | A | 156 | 8.180  | 9.801  | 26.732 | 1.000 | 17.59 |
| ATOM | 1083 | N   | TRP | A | 157 | 10.005 | 10.148 | 25.427 | 1.000 | 20.71 |
| ATOM | 1084 | CA  | TRP | A | 157 | 9.956  | 8.852  | 24.736 | 1.000 | 21.44 |
| ATOM | 1085 | CB  | TRP | A | 157 | 9.852  | 9.047  | 23.221 | 1.000 | 17.84 |
| ATOM | 1086 | CG  | TRP | A | 157 | 11.092 | 9.674  | 22.655 | 1.000 | 22.69 |
| ATOM | 1087 | CD1 | TRP | A | 157 | 12.153 | 9.009  | 22.094 | 1.000 | 24.11 |
| ATOM | 1088 | NE1 | TRP | A | 157 | 13.100 | 9.922  | 21.690 | 1.000 | 23.85 |
| ATOM | 1089 | CE2 | TRP | A | 157 | 12.655 | 11.191 | 21.991 | 1.000 | 20.42 |
| ATOM | 1090 | CD2 | TRP | A | 157 | 11.390 | 11.072 | 22.597 | 1.000 | 18.79 |
| ATOM | 1091 | CE3 | TRP | A | 157 | 10.724 | 12.233 | 22.996 | 1.000 | 18.30 |

**FIGURE 222**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1092 | CZ3 | TRP | A | 157 | 11.325 | 13.459 | 22.787 | 1.000 | 18.73 |
| ATOM | 1093 | CH2 | TRP | A | 157 | 12.582 | 13.548 | 22.179 | 1.000 | 19.11 |
| ATOM | 1094 | CZ2 | TRP | A | 157 | 13.254 | 12.423 | 21.783 | 1.000 | 16.74 |
| ATOM | 1095 | C   | TRP | A | 157 | 11.180 | 8.027  | 25.116 | 1.000 | 21.33 |
| ATOM | 1096 | O   | TRP | A | 157 | 12.146 | 8.606  | 25.626 | 1.000 | 22.55 |
| ATOM | 1097 | N   | PRO | A | 158 | 11.211 | 6.722  | 24.940 | 1.000 | 25.25 |
| ATOM | 1098 | CA  | PRO | A | 158 | 12.363 | 5.904  | 25.331 | 1.000 | 23.55 |
| ATOM | 1099 | CB  | PRO | A | 158 | 11.959 | 4.495  | 24.848 | 1.000 | 23.59 |
| ATOM | 1100 | CG  | PRO | A | 158 | 10.459 | 4.540  | 25.001 | 1.000 | 24.03 |
| ATOM | 1101 | CD  | PRO | A | 158 | 10.115 | 5.887  | 24.391 | 1.000 | 24.42 |
| ATOM | 1102 | C   | PRO | A | 158 | 13.675 | 6.254  | 24.671 | 1.000 | 22.71 |
| ATOM | 1103 | O   | PRO | A | 158 | 13.804 | 6.665  | 23.522 | 1.000 | 24.60 |
| ATOM | 1104 | N   | ALA | A | 159 | 14.735 | 6.052  | 25.470 | 1.000 | 25.38 |
| ATOM | 1105 | CA  | ALA | A | 159 | 16.057 | 6.433  | 24.978 | 1.000 | 26.79 |
| ATOM | 1106 | CB  | ALA | A | 159 | 16.933 | 6.787  | 26.175 | 1.000 | 30.60 |
| ATOM | 1107 | C   | ALA | A | 159 | 16.686 | 5.340  | 24.141 | 1.000 | 31.84 |
| ATOM | 1108 | O   | ALA | A | 159 | 17.702 | 5.599  | 23.481 | 1.000 | 37.52 |
| ATOM | 1109 | N   | ASP | A | 160 | 16.119 | 4.135  | 24.142 | 1.000 | 24.95 |
| ATOM | 1110 | CA  | ASP | A | 160 | 16.648 | 3.021  | 23.361 | 1.000 | 29.97 |
| ATOM | 1111 | CB  | ASP | A | 160 | 17.725 | 2.249  | 24.119 | 1.000 | 33.98 |
| ATOM | 1112 | CG  | ASP | A | 160 | 17.259 | 1.971  | 25.541 | 1.000 | 35.26 |
| ATOM | 1113 | OD1 | ASP | A | 160 | 16.102 | 1.530  | 25.682 | 1.000 | 31.88 |
| ATOM | 1114 | OD2 | ASP | A | 160 | 18.045 | 2.209  | 26.482 | 1.000 | 37.41 |
| ATOM | 1115 | C   | ASP | A | 160 | 15.522 | 2.053  | 23.016 | 1.000 | 28.09 |
| ATOM | 1116 | O   | ASP | A | 160 | 14.364 | 2.428  | 23.164 | 1.000 | 25.87 |
| ATOM | 1117 | N   | GLN | A | 161 | 15.855 | 0.834  | 22.622 | 1.000 | 24.92 |
| ATOM | 1118 | CA  | GLN | A | 161 | 14.765 | -0.040 | 22.162 | 1.000 | 23.89 |
| ATOM | 1119 | CB  | GLN | A | 161 | 15.223 | -0.925 | 20.993 | 1.000 | 30.92 |
| ATOM | 1120 | CG  | GLN | A | 161 | 15.788 | -0.089 | 19.845 | 1.000 | 45.69 |
| ATOM | 1121 | CD  | GLN | A | 161 | 15.671 | -0.678 | 18.458 | 1.000 | 48.73 |
| ATOM | 1122 | OE1 | GLN | A | 161 | 15.341 | -1.845 | 18.249 | 1.000 | 48.46 |
| ATOM | 1123 | NE2 | GLN | A | 161 | 15.952 | 0.136  | 17.441 | 1.000 | 68.57 |
| ATOM | 1124 | C   | GLN | A | 161 | 14.187 | -0.899 | 23.271 | 1.000 | 24.30 |
| ATOM | 1125 | O   | GLN | A | 161 | 13.413 | -1.806 | 22.956 | 1.000 | 25.26 |
| ATOM | 1126 | N   | ASP | A | 162 | 14.518 | -0.604 | 24.521 | 1.000 | 25.88 |
| ATOM | 1127 | CA  | ASP | A | 162 | 13.974 | -1.361 | 25.644 | 1.000 | 27.98 |
| ATOM | 1128 | CB  | ASP | A | 162 | 14.876 | -1.203 | 26.872 | 1.000 | 26.59 |
| ATOM | 1129 | CG  | ASP | A | 162 | 16.207 | -1.921 | 26.713 | 1.000 | 28.66 |
| ATOM | 1130 | OD1 | ASP | A | 162 | 16.491 | -2.448 | 25.628 | 1.000 | 31.96 |
| ATOM | 1131 | OD2 | ASP | A | 162 | 16.968 | -1.953 | 27.694 | 1.000 | 34.72 |
| ATOM | 1132 | C   | ASP | A | 162 | 12.569 | -0.891 | 25.982 | 1.000 | 26.99 |
| ATOM | 1133 | O   | ASP | A | 162 | 12.382 | 0.304  | 26.182 | 1.000 | 27.57 |
| ATOM | 1134 | N   | SER | A | 163 | 11.587 | -1.785 | 26.071 | 1.000 | 22.21 |
| ATOM | 1135 | CA  | SER | A | 163 | 10.208 | -1.323 | 26.297 | 1.000 | 18.32 |
| ATOM | 1136 | CB  | SER | A | 163 | 9.239  | -2.491 | 26.111 | 1.000 | 19.11 |
| ATOM | 1137 | OG  | SER | A | 163 | 9.616  | -3.639 | 26.863 | 1.000 | 24.74 |
| ATOM | 1138 | C   | SER | A | 163 | 10.065 | -0.701 | 27.671 | 1.000 | 19.89 |
| ATOM | 1139 | O   | SER | A | 163 | 10.822 | -1.039 | 28.596 | 1.000 | 23.48 |
| ATOM | 1140 | N   | LEU | A | 164 | 9.115  | 0.215  | 27.839 | 1.000 | 22.10 |
| ATOM | 1141 | CA  | LEU | A | 164 | 8.902  | 0.835  | 29.142 | 1.000 | 25.88 |
| ATOM | 1142 | CB  | LEU | A | 164 | 9.650  | 2.160  | 29.279 | 1.000 | 23.32 |
| ATOM | 1143 | CG  | LEU | A | 164 | 11.081 | 2.263  | 29.771 | 1.000 | 32.69 |

**FIGURE 223**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1144 | CD1 | LEU | A | 164 | 11.536 | 3.726  | 29.711 | 1.000 | 28.59 |
| ATOM | 1145 | CD2 | LEU | A | 164 | 11.280 | 1.731  | 31.183 | 1.000 | 31.11 |
| ATOM | 1146 | C   | LEU | A | 164 | 7.421  | 1.126  | 29.396 | 1.000 | 27.10 |
| ATOM | 1147 | O   | LEU | A | 164 | 6.712  | 1.554  | 28.476 | 1.000 | 18.26 |
| ATOM | 1148 | N   | TYR | A | 165 | 6.948  | 0.930  | 30.633 | 1.000 | 16.81 |
| ATOM | 1149 | CA  | TYR | A | 165 | 5.610  | 1.374  | 30.989 | 1.000 | 15.66 |
| ATOM | 1150 | CB  | TYR | A | 165 | 5.152  | 0.803  | 32.324 | 1.000 | 17.16 |
| ATOM | 1151 | CG  | TYR | A | 165 | 4.704  | -0.642 | 32.238 | 1.000 | 22.22 |
| ATOM | 1152 | CD1 | TYR | A | 165 | 3.479  | -0.947 | 31.670 | 1.000 | 22.09 |
| ATOM | 1153 | CE1 | TYR | A | 165 | 3.008  | -2.244 | 31.568 | 1.000 | 21.78 |
| ATOM | 1154 | CZ  | TYR | A | 165 | 3.812  | -3.256 | 32.062 | 1.000 | 20.60 |
| ATOM | 1155 | OH  | TYR | A | 165 | 3.338  | -4.550 | 31.950 | 1.000 | 25.51 |
| ATOM | 1156 | CE2 | TYR | A | 165 | 5.032  | -2.978 | 32.631 | 1.000 | 18.30 |
| ATOM | 1157 | CD2 | TYR | A | 165 | 5.506  | -1.670 | 32.740 | 1.000 | 18.57 |
| ATOM | 1158 | C   | TYR | A | 165 | 5.563  | 2.905  | 31.134 | 1.000 | 20.90 |
| ATOM | 1159 | O   | TYR | A | 165 | 6.525  | 3.443  | 31.688 | 1.000 | 19.46 |
| ATOM | 1160 | N   | TYR | A | 166 | 4.495  | 3.530  | 30.690 | 1.000 | 17.57 |
| ATOM | 1161 | CA  | TYR | A | 166 | 4.172  | 4.933  | 30.964 | 1.000 | 16.74 |
| ATOM | 1162 | CB  | TYR | A | 166 | 4.262  | 5.809  | 29.718 | 1.000 | 17.74 |
| ATOM | 1163 | CG  | TYR | A | 166 | 5.648  | 6.083  | 29.202 | 1.000 | 18.55 |
| ATOM | 1164 | CD1 | TYR | A | 166 | 6.318  | 7.284  | 29.472 | 1.000 | 15.85 |
| ATOM | 1165 | CE1 | TYR | A | 166 | 7.589  | 7.509  | 28.990 | 1.000 | 15.83 |
| ATOM | 1166 | CZ  | TYR | A | 166 | 8.236  | 6.569  | 28.235 | 1.000 | 17.11 |
| ATOM | 1167 | OH  | TYR | A | 166 | 9.498  | 6.772  | 27.739 | 1.000 | 21.34 |
| ATOM | 1168 | CE2 | TYR | A | 166 | 7.597  | 5.380  | 27.954 | 1.000 | 20.45 |
| ATOM | 1169 | CD2 | TYR | A | 166 | 6.324  | 5.153  | 28.434 | 1.000 | 19.30 |
| ATOM | 1170 | C   | TYR | A | 166 | 2.755  | 4.969  | 31.521 | 1.000 | 17.54 |
| ATOM | 1171 | O   | TYR | A | 166 | 1.784  | 4.874  | 30.773 | 1.000 | 18.04 |
| ATOM | 1172 | N   | GLY | A | 167 | 2.582  | 5.076  | 32.829 | 1.000 | 18.81 |
| ATOM | 1173 | CA  | GLY | A | 167 | 1.205  | 4.954  | 33.330 | 1.000 | 22.60 |
| ATOM | 1174 | C   | GLY | A | 167 | 0.691  | 3.555  | 33.040 | 1.000 | 22.40 |
| ATOM | 1175 | O   | GLY | A | 167 | 1.404  | 2.570  | 33.233 | 1.000 | 24.80 |
| ATOM | 1176 | N   | ASP | A | 168 | -0.529 | 3.434  | 32.527 | 1.000 | 21.14 |
| ATOM | 1177 | CA  | ASP | A | 168 | -1.052 | 2.125  | 32.187 | 1.000 | 19.46 |
| ATOM | 1178 | CB  | ASP | A | 168 | -2.583 | 2.105  | 32.330 | 1.000 | 19.01 |
| ATOM | 1179 | CG  | ASP | A | 168 | -2.972 | 2.233  | 33.792 | 1.000 | 29.38 |
| ATOM | 1180 | OD1 | ASP | A | 168 | -2.199 | 1.795  | 34.675 | 1.000 | 31.79 |
| ATOM | 1181 | OD2 | ASP | A | 168 | -4.064 | 2.776  | 34.047 | 1.000 | 41.21 |
| ATOM | 1182 | C   | ASP | A | 168 | -0.707 | 1.690  | 30.779 | 1.000 | 22.83 |
| ATOM | 1183 | O   | ASP | A | 168 | -1.223 | 0.665  | 30.330 | 1.000 | 32.53 |
| ATOM | 1184 | N   | LEU | A | 169 | 0.113  | 2.428  | 30.059 | 1.000 | 22.05 |
| ATOM | 1185 | CA  | LEU | A | 169 | 0.439  | 2.054  | 28.685 | 1.000 | 20.08 |
| ATOM | 1186 | CB  | LEU | A | 169 | 0.372  | 3.268  | 27.736 | 1.000 | 19.68 |
| ATOM | 1187 | CG  | LEU | A | 169 | -0.925 | 4.075  | 27.798 | 1.000 | 38.06 |
| ATOM | 1188 | CD1 | LEU | A | 169 | -0.792 | 5.463  | 27.170 | 1.000 | 25.80 |
| ATOM | 1189 | CD2 | LEU | A | 169 | -2.049 | 3.304  | 27.119 | 1.000 | 37.43 |
| ATOM | 1190 | C   | LEU | A | 169 | 1.840  | 1.480  | 28.619 | 1.000 | 21.18 |
| ATOM | 1191 | O   | LEU | A | 169 | 2.677  | 1.776  | 29.476 | 1.000 | 22.88 |
| ATOM | 1192 | N   | ILE | A | 170 | 2.110  | 0.675  | 27.585 | 1.000 | 15.34 |
| ATOM | 1193 | CA  | ILE | A | 170 | 3.498  | 0.257  | 27.438 | 1.000 | 16.78 |
| ATOM | 1194 | CB  | ILE | A | 170 | 3.759  | -1.248 | 27.605 | 1.000 | 23.77 |
| ATOM | 1195 | CG1 | ILE | A | 170 | 5.235  | -1.602 | 27.342 | 1.000 | 28.45 |

FIGURE 224

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1196 | CD1 | ILE | A | 170 | 5.709  | -2.782 | 28.165 | 1.000 | 28.18 |
| ATOM | 1197 | CG2 | ILE | A | 170 | 2.849  | -2.102 | 26.746 | 1.000 | 23.17 |
| ATOM | 1198 | C   | ILE | A | 170 | 3.966  | 0.706  | 26.047 | 1.000 | 19.57 |
| ATOM | 1199 | O   | ILE | A | 170 | 3.177  | 0.625  | 25.107 | 1.000 | 18.10 |
| ATOM | 1200 | N   | LEU | A | 171 | 5.196  | 1.186  | 26.013 | 1.000 | 19.57 |
| ATOM | 1201 | CA  | LEU | A | 171 | 5.709  | 1.829  | 24.789 | 1.000 | 23.46 |
| ATOM | 1202 | CB  | LEU | A | 171 | 5.723  | 3.318  | 25.102 | 1.000 | 24.58 |
| ATOM | 1203 | CG  | LEU | A | 171 | 6.059  | 4.395  | 24.098 | 1.000 | 38.61 |
| ATOM | 1204 | CD1 | LEU | A | 171 | 4.995  | 4.543  | 23.027 | 1.000 | 29.72 |
| ATOM | 1205 | CD2 | LEU | A | 171 | 6.247  | 5.726  | 24.826 | 1.000 | 32.91 |
| ATOM | 1206 | C   | LEU | A | 171 | 7.042  | 1.210  | 24.442 | 1.000 | 25.87 |
| ATOM | 1207 | O   | LEU | A | 171 | 7.863  | 0.848  | 25.294 | 1.000 | 22.43 |
| ATOM | 1208 | N   | GLN | A | 172 | 7.320  | 1.018  | 23.159 | 1.000 | 18.94 |
| ATOM | 1209 | CA  | GLN | A | 172 | 8.609  | 0.485  | 22.749 | 1.000 | 18.74 |
| ATOM | 1210 | CB  | GLN | A | 172 | 8.516  | -1.033 | 22.548 | 1.000 | 25.07 |
| ATOM | 1211 | CG  | GLN | A | 172 | 9.801  | -1.733 | 22.146 | 1.000 | 23.89 |
| ATOM | 1212 | CD  | GLN | A | 172 | 9.639  | -3.222 | 21.918 | 1.000 | 32.82 |
| ATOM | 1213 | OE1 | GLN | A | 172 | 8.737  | -3.720 | 21.242 | 1.000 | 36.92 |
| ATOM | 1214 | NE2 | GLN | A | 172 | 10.552 | -3.981 | 22.530 | 1.000 | 34.84 |
| ATOM | 1215 | C   | GLN | A | 172 | 9.049  | 1.190  | 21.475 | 1.000 | 20.94 |
| ATOM | 1216 | O   | GLN | A | 172 | 8.271  | 1.224  | 20.521 | 1.000 | 27.01 |
| ATOM | 1217 | N   | MET | A | 173 | 10.265 | 1.709  | 21.448 | 1.000 | 21.76 |
| ATOM | 1218 | CA  | MET | A | 173 | 10.771 | 2.361  | 20.246 | 1.000 | 19.32 |
| ATOM | 1219 | CB  | MET | A | 173 | 11.848 | 3.393  | 20.622 | 1.000 | 20.29 |
| ATOM | 1220 | CG  | MET | A | 173 | 12.395 | 4.082  | 19.350 | 1.000 | 23.01 |
| ATOM | 1221 | SD  | MET | A | 173 | 13.333 | 5.573  | 19.752 | 1.000 | 23.47 |
| ATOM | 1222 | CE  | MET | A | 173 | 14.788 | 4.835  | 20.498 | 1.000 | 34.32 |
| ATOM | 1223 | C   | MET | A | 173 | 11.331 | 1.325  | 19.286 | 1.000 | 21.94 |
| ATOM | 1224 | O   | MET | A | 173 | 12.211 | 0.554  | 19.678 | 1.000 | 25.02 |
| ATOM | 1225 | N   | LEU | A | 174 | 10.824 | 1.300  | 18.058 | 1.000 | 21.94 |
| ATOM | 1226 | CA  | LEU | A | 174 | 11.188 | 0.272  | 17.086 | 1.000 | 26.84 |
| ATOM | 1227 | CB  | LEU | A | 174 | 9.993  | -0.104 | 16.224 | 1.000 | 29.19 |
| ATOM | 1228 | CG  | LEU | A | 174 | 8.732  | -0.590 | 16.934 | 1.000 | 33.01 |
| ATOM | 1229 | CD1 | LEU | A | 174 | 7.688  | -0.964 | 15.897 | 1.000 | 29.01 |
| ATOM | 1230 | CD2 | LEU | A | 174 | 9.062  | -1.757 | 17.857 | 1.000 | 38.21 |
| ATOM | 1231 | C   | LEU | A | 174 | 12.299 | 0.737  | 16.159 | 1.000 | 27.31 |
| ATOM | 1232 | O   | LEU | A | 174 | 13.081 | -0.049 | 15.641 | 1.000 | 28.22 |
| ATOM | 1233 | N   | SER | A | 175 | 12.364 | 2.050  | 15.956 | 1.000 | 28.86 |
| ATOM | 1234 | CA  | SER | A | 175 | 13.420 | 2.612  | 15.111 | 1.000 | 30.23 |
| ATOM | 1235 | CB  | SER | A | 175 | 13.135 | 2.372  | 13.626 | 1.000 | 29.79 |
| ATOM | 1236 | OG  | SER | A | 175 | 12.320 | 3.403  | 13.111 | 1.000 | 28.04 |
| ATOM | 1237 | C   | SER | A | 175 | 13.595 | 4.101  | 15.397 | 1.000 | 22.48 |
| ATOM | 1238 | O   | SER | A | 175 | 12.690 | 4.787  | 15.885 | 1.000 | 22.47 |
| ATOM | 1239 | N   | GLU | A | 176 | 14.798 | 4.562  | 15.104 | 1.000 | 20.99 |
| ATOM | 1240 | CA  | GLU | A | 176 | 15.204 | 5.939  | 15.322 | 1.000 | 21.52 |
| ATOM | 1241 | CB  | GLU | A | 176 | 15.885 | 6.109  | 16.674 | 1.000 | 18.41 |
| ATOM | 1242 | CG  | GLU | A | 176 | 16.366 | 7.514  | 16.976 | 1.000 | 22.49 |
| ATOM | 1243 | CD  | GLU | A | 176 | 16.890 | 7.563  | 18.413 | 1.000 | 39.47 |
| ATOM | 1244 | OE1 | GLU | A | 176 | 18.041 | 7.104  | 18.596 | 1.000 | 35.29 |
| ATOM | 1245 | OE2 | GLU | A | 176 | 16.182 | 8.023  | 19.331 | 1.000 | 26.84 |
| ATOM | 1246 | C   | GLU | A | 176 | 16.158 | 6.334  | 14.203 | 1.000 | 35.39 |
| ATOM | 1247 | O   | GLU | A | 176 | 17.237 | 5.756  | 14.149 | 1.000 | 26.11 |

**FIGURE 225**

|      |      |     |           |        |        |        |       |       |
|------|------|-----|-----------|--------|--------|--------|-------|-------|
| ATOM | 1248 | N   | SER A 177 | 15.754 | 7.260  | 13.341 | 1.000 | 26.10 |
| ATOM | 1249 | CA  | SER A 177 | 16.562 | 7.596  | 12.175 | 1.000 | 22.13 |
| ATOM | 1250 | CB  | SER A 177 | 15.850 | 7.215  | 10.880 | 1.000 | 24.63 |
| ATOM | 1251 | OG  | SER A 177 | 15.442 | 5.858  | 10.852 | 1.000 | 32.57 |
| ATOM | 1252 | C   | SER A 177 | 16.888 | 9.079  | 12.211 | 1.000 | 19.74 |
| ATOM | 1253 | O   | SER A 177 | 16.041 | 9.955  | 12.003 | 1.000 | 24.72 |
| ATOM | 1254 | N   | VAL A 178 | 18.142 | 9.387  | 12.521 | 1.000 | 21.76 |
| ATOM | 1255 | CA  | VAL A 178 | 18.577 | 10.766 | 12.651 | 1.000 | 20.70 |
| ATOM | 1256 | CB  | VAL A 178 | 19.777 | 10.890 | 13.604 | 1.000 | 30.20 |
| ATOM | 1257 | CG1 | VAL A 178 | 20.138 | 12.353 | 13.823 | 1.000 | 22.39 |
| ATOM | 1258 | CG2 | VAL A 178 | 19.478 | 10.224 | 14.943 | 1.000 | 30.74 |
| ATOM | 1259 | C   | VAL A 178 | 18.959 | 11.311 | 11.280 | 1.000 | 27.01 |
| ATOM | 1260 | O   | VAL A 178 | 19.885 | 10.794 | 10.652 | 1.000 | 26.60 |
| ATOM | 1261 | N   | LEU A 179 | 18.244 | 12.333 | 10.828 | 1.000 | 23.24 |
| ATOM | 1262 | CA  | LEU A 179 | 18.550 | 12.947 | 9.541  | 1.000 | 17.95 |
| ATOM | 1263 | CB  | LEU A 179 | 17.292 | 12.950 | 8.668  | 1.000 | 19.90 |
| ATOM | 1264 | CG  | LEU A 179 | 16.414 | 11.712 | 8.694  | 1.000 | 19.48 |
| ATOM | 1265 | CD1 | LEU A 179 | 15.201 | 11.861 | 7.765  | 1.000 | 20.09 |
| ATOM | 1266 | CD2 | LEU A 179 | 17.209 | 10.467 | 8.304  | 1.000 | 23.69 |
| ATOM | 1267 | C   | LEU A 179 | 19.119 | 14.337 | 9.791  | 1.000 | 22.68 |
| ATOM | 1268 | O   | LEU A 179 | 19.079 | 14.824 | 10.939 | 1.000 | 23.34 |
| ATOM | 1269 | N   | PRO A 180 | 19.677 | 15.022 | 8.798  | 1.000 | 26.71 |
| ATOM | 1270 | CA  | PRO A 180 | 20.320 | 16.317 | 9.086  | 1.000 | 23.99 |
| ATOM | 1271 | CB  | PRO A 180 | 20.700 | 16.849 | 7.686  | 1.000 | 24.76 |
| ATOM | 1272 | CG  | PRO A 180 | 20.859 | 15.612 | 6.863  | 1.000 | 30.87 |
| ATOM | 1273 | CD  | PRO A 180 | 19.801 | 14.649 | 7.378  | 1.000 | 29.95 |
| ATOM | 1274 | C   | PRO A 180 | 19.439 | 17.339 | 9.771  | 1.000 | 23.60 |
| ATOM | 1275 | O   | PRO A 180 | 19.901 | 18.080 | 10.636 | 1.000 | 22.88 |
| ATOM | 1276 | N   | GLU A 181 | 18.151 | 17.441 | 9.439  | 1.000 | 21.19 |
| ATOM | 1277 | CA  | GLU A 181 | 17.363 | 18.480 | 10.078 | 1.000 | 21.28 |
| ATOM | 1278 | CB  | GLU A 181 | 16.858 | 19.455 | 8.991  | 1.000 | 24.45 |
| ATOM | 1279 | CG  | GLU A 181 | 18.003 | 20.315 | 8.476  | 1.000 | 34.87 |
| ATOM | 1280 | CD  | GLU A 181 | 17.596 | 21.325 | 7.421  | 1.000 | 37.86 |
| ATOM | 1281 | OE1 | GLU A 181 | 16.746 | 21.008 | 6.567  | 1.000 | 32.02 |
| ATOM | 1282 | OE2 | GLU A 181 | 18.154 | 22.440 | 7.452  | 1.000 | 44.17 |
| ATOM | 1283 | C   | GLU A 181 | 16.178 | 17.945 | 10.870 | 1.000 | 17.99 |
| ATOM | 1284 | O   | GLU A 181 | 15.507 | 18.740 | 11.537 | 1.000 | 19.13 |
| ATOM | 1285 | N   | TRP A 182 | 15.906 | 16.648 | 10.817 | 1.000 | 23.72 |
| ATOM | 1286 | CA  | TRP A 182 | 14.848 | 16.095 | 11.672 | 1.000 | 20.93 |
| ATOM | 1287 | CB  | TRP A 182 | 13.432 | 16.217 | 11.113 | 1.000 | 15.09 |
| ATOM | 1288 | CG  | TRP A 182 | 13.192 | 15.913 | 9.681  | 1.000 | 16.03 |
| ATOM | 1289 | CD1 | TRP A 182 | 12.852 | 14.727 | 9.123  | 1.000 | 20.35 |
| ATOM | 1290 | NE1 | TRP A 182 | 12.715 | 14.821 | 7.763  | 1.000 | 23.86 |
| ATOM | 1291 | CE2 | TRP A 182 | 12.971 | 16.112 | 7.407  | 1.000 | 15.42 |
| ATOM | 1292 | CD2 | TRP A 182 | 13.275 | 16.826 | 8.568  | 1.000 | 18.32 |
| ATOM | 1293 | CE3 | TRP A 182 | 13.583 | 18.197 | 8.484  | 1.000 | 18.38 |
| ATOM | 1294 | CZ3 | TRP A 182 | 13.571 | 18.785 | 7.229  | 1.000 | 19.84 |
| ATOM | 1295 | CH2 | TRP A 182 | 13.261 | 18.032 | 6.085  | 1.000 | 21.10 |
| ATOM | 1296 | CZ2 | TRP A 182 | 12.956 | 16.698 | 6.134  | 1.000 | 18.37 |
| ATOM | 1297 | C   | TRP A 182 | 15.188 | 14.629 | 11.929 | 1.000 | 21.61 |
| ATOM | 1298 | O   | TRP A 182 | 15.996 | 14.011 | 11.228 | 1.000 | 21.72 |
| ATOM | 1299 | N   | THR A 183 | 14.549 | 14.085 | 12.961 | 1.000 | 18.39 |

**FIGURE 226**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1300 | CA  | THR | A | 183 | 14.699 | 12.677 | 13.292 | 1.000 | 20.50 |
| ATOM | 1301 | CB  | THR | A | 183 | 15.328 | 12.553 | 14.701 | 1.000 | 23.44 |
| ATOM | 1302 | OG1 | THR | A | 183 | 16.636 | 13.143 | 14.619 | 1.000 | 24.00 |
| ATOM | 1303 | CG2 | THR | A | 183 | 15.453 | 11.104 | 15.137 | 1.000 | 21.54 |
| ATOM | 1304 | C   | THR | A | 183 | 13.349 | 11.988 | 13.226 | 1.000 | 16.48 |
| ATOM | 1305 | O   | THR | A | 183 | 12.354 | 12.543 | 13.710 | 1.000 | 18.87 |
| ATOM | 1306 | N   | ILE | A | 184 | 13.301 | 10.809 | 12.641 | 1.000 | 15.19 |
| ATOM | 1307 | CA  | ILE | A | 184 | 12.051 | 10.059 | 12.556 | 1.000 | 15.66 |
| ATOM | 1308 | CB  | ILE | A | 184 | 11.775 | 9.676  | 11.096 | 1.000 | 19.83 |
| ATOM | 1309 | CG1 | ILE | A | 184 | 11.821 | 10.921 | 10.196 | 1.000 | 20.74 |
| ATOM | 1310 | CD1 | ILE | A | 184 | 11.379 | 10.717 | 8.765  | 1.000 | 23.01 |
| ATOM | 1311 | CG2 | ILE | A | 184 | 10.481 | 8.900  | 10.978 | 1.000 | 19.48 |
| ATOM | 1312 | C   | ILE | A | 184 | 12.134 | 8.828  | 13.450 | 1.000 | 25.32 |
| ATOM | 1313 | O   | ILE | A | 184 | 13.056 | 8.018  | 13.311 | 1.000 | 28.73 |
| ATOM | 1314 | N   | ARG | A | 185 | 11.189 | 8.678  | 14.370 | 1.000 | 21.95 |
| ATOM | 1315 | CA  | ARG | A | 185 | 11.171 | 7.501  | 15.231 | 1.000 | 19.00 |
| ATOM | 1316 | CB  | ARG | A | 185 | 11.381 | 7.882  | 16.693 | 1.000 | 17.64 |
| ATOM | 1317 | CG  | ARG | A | 185 | 12.739 | 8.478  | 17.011 | 1.000 | 22.12 |
| ATOM | 1318 | CD  | ARG | A | 185 | 12.764 | 9.060  | 18.407 | 1.000 | 22.23 |
| ATOM | 1319 | NE  | ARG | A | 185 | 13.977 | 9.765  | 18.768 | 1.000 | 27.88 |
| ATOM | 1320 | CZ  | ARG | A | 185 | 14.318 | 11.031 | 18.624 | 1.000 | 22.96 |
| ATOM | 1321 | NH1 | ARG | A | 185 | 13.515 | 11.930 | 18.062 | 1.000 | 21.31 |
| ATOM | 1322 | NH2 | ARG | A | 185 | 15.513 | 11.426 | 19.056 | 1.000 | 28.28 |
| ATOM | 1323 | C   | ARG | A | 185 | 9.836  | 6.796  | 15.067 | 1.000 | 20.34 |
| ATOM | 1324 | O   | ARG | A | 185 | 8.827  | 7.415  | 14.740 | 1.000 | 19.60 |
| ATOM | 1325 | N   | GLU | A | 186 | 9.842  | 5.499  | 15.318 | 1.000 | 21.83 |
| ATOM | 1326 | CA  | GLU | A | 186 | 8.590  | 4.756  | 15.330 | 1.000 | 19.84 |
| ATOM | 1327 | CB  | GLU | A | 186 | 8.495  | 3.779  | 14.165 | 1.000 | 27.08 |
| ATOM | 1328 | CG  | GLU | A | 186 | 7.086  | 3.286  | 13.877 | 1.000 | 38.65 |
| ATOM | 1329 | CD  | GLU | A | 186 | 6.961  | 2.255  | 12.778 | 1.000 | 49.85 |
| ATOM | 1330 | OE1 | GLU | A | 186 | 7.958  | 1.554  | 12.481 | 1.000 | 59.07 |
| ATOM | 1331 | OE2 | GLU | A | 186 | 5.874  | 2.119  | 12.169 | 1.000 | 41.81 |
| ATOM | 1332 | C   | GLU | A | 186 | 8.507  | 4.004  | 16.664 | 1.000 | 24.47 |
| ATOM | 1333 | O   | GLU | A | 186 | 9.494  | 3.391  | 17.085 | 1.000 | 28.68 |
| ATOM | 1334 | N   | PHE | A | 187 | 7.342  | 4.092  | 17.281 | 1.000 | 21.26 |
| ATOM | 1335 | CA  | PHE | A | 187 | 7.016  | 3.401  | 18.513 | 1.000 | 17.58 |
| ATOM | 1336 | CB  | PHE | A | 187 | 6.609  | 4.390  | 19.609 | 1.000 | 19.02 |
| ATOM | 1337 | CG  | PHE | A | 187 | 7.601  | 5.542  | 19.741 | 1.000 | 26.16 |
| ATOM | 1338 | CD1 | PHE | A | 187 | 7.288  | 6.798  | 19.268 | 1.000 | 22.44 |
| ATOM | 1339 | CE1 | PHE | A | 187 | 8.192  | 7.832  | 19.409 | 1.000 | 30.77 |
| ATOM | 1340 | CZ  | PHE | A | 187 | 9.428  | 7.634  | 19.993 | 1.000 | 26.12 |
| ATOM | 1341 | CE2 | PHE | A | 187 | 9.746  | 6.376  | 20.477 | 1.000 | 27.12 |
| ATOM | 1342 | CD2 | PHE | A | 187 | 8.832  | 5.341  | 20.350 | 1.000 | 25.25 |
| ATOM | 1343 | C   | PHE | A | 187 | 5.836  | 2.453  | 18.339 | 1.000 | 20.12 |
| ATOM | 1344 | O   | PHE | A | 187 | 4.844  | 2.733  | 17.687 | 1.000 | 23.02 |
| ATOM | 1345 | N   | LYS | A | 188 | 5.969  | 1.320  | 19.015 | 1.000 | 29.00 |
| ATOM | 1346 | CA  | LYS | A | 188 | 4.814  | 0.486  | 19.315 | 1.000 | 23.44 |
| ATOM | 1347 | CB  | LYS | A | 188 | 5.229  | -0.986 | 19.280 | 1.000 | 29.53 |
| ATOM | 1348 | CG  | LYS | A | 188 | 4.064  | -1.959 | 19.180 | 1.000 | 41.78 |
| ATOM | 1349 | CD  | LYS | A | 188 | 4.560  | -3.360 | 18.830 | 1.000 | 46.50 |
| ATOM | 1350 | CE  | LYS | A | 188 | 5.255  | -3.976 | 20.036 | 1.000 | 45.29 |
| ATOM | 1351 | NZ  | LYS | A | 188 | 5.958  | -5.246 | 19.707 | 1.000 | 51.18 |

**FIGURE 227**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |         |        |        |       |        |
|------|------|-----|-----|---|-----|---------|--------|--------|-------|--------|
| ATOM | 1352 | C   | LYS | A | 188 | 4.247   | 0.908  | 20.669 | 1.000 | 21.37  |
| ATOM | 1353 | O   | LYS | A | 188 | 4.984   | 1.012  | 21.650 | 1.000 | 20.70  |
| ATOM | 1354 | N   | ILE | A | 189 | 2.942   | 1.151  | 20.722 | 1.000 | 19.68  |
| ATOM | 1355 | CA  | ILE | A | 189 | 2.280   | 1.419  | 21.990 | 1.000 | 20.68  |
| ATOM | 1356 | CB  | ILE | A | 189 | 1.712   | 2.853  | 22.019 | 1.000 | 26.52  |
| ATOM | 1357 | CG1 | ILE | A | 189 | 1.092   | 3.235  | 23.363 | 1.000 | 22.26  |
| ATOM | 1358 | CD1 | ILE | A | 189 | 0.940   | 4.748  | 23.485 | 1.000 | 39.28  |
| ATOM | 1359 | CG2 | ILE | A | 189 | 0.721   | 3.104  | 20.879 | 1.000 | 26.76  |
| ATOM | 1360 | C   | ILE | A | 189 | 1.160   | 0.429  | 22.259 | 1.000 | 25.87  |
| ATOM | 1361 | O   | ILE | A | 189 | 0.397   | 0.070  | 21.351 | 1.000 | 23.56  |
| ATOM | 1362 | N   | CYS | A | 190 | 1.032   | -0.021 | 23.514 | 1.000 | 24.27  |
| ATOM | 1363 | CA  | CYS | A | 190 | -0.078  | -0.912 | 23.859 | 1.000 | 21.00  |
| ATOM | 1364 | CB  | CYS | A | 190 | 0.402   | -2.336 | 24.179 | 1.000 | 28.92  |
| ATOM | 1365 | SG  | CYS | A | 190 | 1.318   | -3.174 | 22.867 | 1.000 | 32.32  |
| ATOM | 1366 | C   | CYS | A | 190 | -0.838  | -0.365 | 25.055 | 1.000 | 26.90  |
| ATOM | 1367 | O   | CYS | A | 190 | -0.279  | -0.024 | 26.098 | 1.000 | 22.81  |
| ATOM | 1368 | N   | GLY | A | 191 | -2.159  | -0.270 | 24.946 | 1.000 | 28.18  |
| ATOM | 1369 | CA  | GLY | A | 191 | -2.883  | 0.291  | 26.094 | 1.000 | 35.73  |
| ATOM | 1370 | C   | GLY | A | 191 | -4.150  | -0.485 | 26.348 | 1.000 | 42.74  |
| ATOM | 1371 | O   | GLY | A | 191 | -4.326  | -1.578 | 25.793 | 1.000 | 32.85  |
| ATOM | 1372 | N   | GLU | A | 192 | -5.093  | -0.003 | 27.180 | 1.000 | 51.55  |
| ATOM | 1373 | CA  | GLU | A | 192 | -6.223  | -0.938 | 27.283 | 1.000 | 66.18  |
| ATOM | 1374 | CB  | GLU | A | 192 | -7.133  | -0.742 | 28.489 | 1.000 | 76.10  |
| ATOM | 1375 | CG  | GLU | A | 192 | -7.860  | -2.067 | 28.785 | 1.000 | 85.72  |
| ATOM | 1376 | CD  | GLU | A | 192 | -7.026  | -3.266 | 28.356 | 1.000 | 87.86  |
| ATOM | 1377 | OE1 | GLU | A | 192 | -6.184  | -3.687 | 29.190 | 1.000 | 106.89 |
| ATOM | 1378 | OE2 | GLU | A | 192 | -7.174  | -3.794 | 27.229 | 1.000 | 63.79  |
| ATOM | 1379 | C   | GLU | A | 192 | -7.019  | -0.844 | 25.974 | 1.000 | 60.51  |
| ATOM | 1380 | O   | GLU | A | 192 | -7.455  | 0.251  | 25.638 | 1.000 | 49.89  |
| ATOM | 1381 | N   | GLU | A | 193 | -7.112  | -1.996 | 25.326 | 1.000 | 57.69  |
| ATOM | 1382 | CA  | GLU | A | 193 | -7.600  | -2.127 | 23.973 | 1.000 | 58.03  |
| ATOM | 1383 | CB  | GLU | A | 193 | -7.726  | -3.604 | 23.546 | 1.000 | 59.99  |
| ATOM | 1384 | CG  | GLU | A | 193 | -8.209  | -3.661 | 22.102 | 1.000 | 70.62  |
| ATOM | 1385 | CD  | GLU | A | 193 | -8.606  | -5.058 | 21.671 | 1.000 | 69.93  |
| ATOM | 1386 | OE1 | GLU | A | 193 | -9.439  | -5.674 | 22.369 | 1.000 | 80.76  |
| ATOM | 1387 | OE2 | GLU | A | 193 | -8.081  | -5.511 | 20.636 | 1.000 | 63.90  |
| ATOM | 1388 | C   | GLU | A | 193 | -8.963  | -1.475 | 23.781 | 1.000 | 64.42  |
| ATOM | 1389 | O   | GLU | A | 193 | -9.945  | -1.868 | 24.403 | 1.000 | 100.70 |
| ATOM | 1390 | N   | GLN | A | 194 | -9.008  | -0.492 | 22.895 | 1.000 | 65.44  |
| ATOM | 1391 | CA  | GLN | A | 194 | -10.257 | 0.128  | 22.460 | 1.000 | 65.33  |
| ATOM | 1392 | CB  | GLN | A | 194 | -10.256 | 1.622  | 22.773 | 1.000 | 59.27  |
| ATOM | 1393 | CG  | GLN | A | 194 | -8.915  | 2.066  | 23.359 | 1.000 | 64.93  |
| ATOM | 1394 | CD  | GLN | A | 194 | -8.739  | 3.571  | 23.383 | 1.000 | 63.48  |
| ATOM | 1395 | OE1 | GLN | A | 194 | -8.193  | 4.160  | 22.449 | 1.000 | 39.84  |
| ATOM | 1396 | NE2 | GLN | A | 194 | -9.206  | 4.183  | 24.467 | 1.000 | 72.21  |
| ATOM | 1397 | C   | GLN | A | 194 | -10.409 | -0.139 | 20.964 | 1.000 | 65.87  |
| ATOM | 1398 | O   | GLN | A | 194 | -10.725 | -1.270 | 20.581 | 1.000 | 56.74  |
| ATOM | 1399 | N   | LEU | A | 195 | -10.151 | 0.891  | 20.161 | 1.000 | 58.59  |
| ATOM | 1400 | CA  | LEU | A | 195 | -10.167 | 0.734  | 18.707 | 1.000 | 53.57  |
| ATOM | 1401 | CB  | LEU | A | 195 | -10.095 | 2.103  | 18.027 | 1.000 | 34.01  |
| ATOM | 1402 | CG  | LEU | A | 195 | -11.473 | 2.711  | 17.749 | 1.000 | 52.84  |
| ATOM | 1403 | CD1 | LEU | A | 195 | -11.369 | 4.144  | 17.248 | 1.000 | 64.31  |

**FIGURE 228**



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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |         |        |        |       |       |
|------|------|-----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 1404 | CD2 | LEU | A | 195 | -12.213 | 1.828  | 16.745 | 1.000 | 77.61 |
| ATOM | 1405 | C   | LEU | A | 195 | -9.029  | -0.175 | 18.251 | 1.000 | 62.19 |
| ATOM | 1406 | O   | LEU | A | 195 | -9.207  | -0.990 | 17.345 | 1.000 | 74.97 |
| ATOM | 1407 | N   | ASP | A | 196 | -7.874  | -0.040 | 18.893 | 1.000 | 64.63 |
| ATOM | 1408 | CA  | ASP | A | 196 | -6.730  | -0.907 | 18.651 | 1.000 | 71.88 |
| ATOM | 1409 | CB  | ASP | A | 196 | -5.616  | -0.149 | 17.929 | 1.000 | 69.22 |
| ATOM | 1410 | CG  | ASP | A | 196 | -5.589  | 1.331  | 18.254 | 1.000 | 68.85 |
| ATOM | 1411 | OD1 | ASP | A | 196 | -5.984  | 1.716  | 19.374 | 1.000 | 46.56 |
| ATOM | 1412 | OD2 | ASP | A | 196 | -5.168  | 2.105  | 17.363 | 1.000 | 68.77 |
| ATOM | 1413 | C   | ASP | A | 196 | -6.197  | -1.496 | 19.959 | 1.000 | 75.55 |
| ATOM | 1414 | O   | ASP | A | 196 | -6.396  | -0.908 | 21.026 | 1.000 | 52.97 |
| ATOM | 1415 | N   | ALA | A | 197 | -5.530  | -2.643 | 19.864 | 1.000 | 77.66 |
| ATOM | 1416 | CA  | ALA | A | 197 | -4.895  | -3.267 | 21.020 | 1.000 | 76.86 |
| ATOM | 1417 | CB  | ALA | A | 197 | -5.256  | -4.738 | 21.113 | 1.000 | 89.29 |
| ATOM | 1418 | C   | ALA | A | 197 | -3.376  | -3.077 | 20.976 | 1.000 | 70.52 |
| ATOM | 1419 | O   | ALA | A | 197 | -2.709  | -3.074 | 22.013 | 1.000 | 40.24 |
| ATOM | 1420 | N   | HIS | A | 198 | -2.852  | -2.910 | 19.772 | 1.000 | 66.05 |
| ATOM | 1421 | CA  | HIS | A | 198 | -1.497  | -2.444 | 19.510 | 1.000 | 70.91 |
| ATOM | 1422 | CB  | HIS | A | 198 | -0.565  | -3.597 | 19.162 | 1.000 | 75.50 |
| ATOM | 1423 | CG  | HIS | A | 198 | -1.090  | -4.481 | 18.069 | 1.000 | 88.48 |
| ATOM | 1424 | ND1 | HIS | A | 198 | -1.492  | -5.779 | 18.290 | 1.000 | 94.26 |
| ATOM | 1425 | CE1 | HIS | A | 198 | -1.906  | -6.315 | 17.155 | 1.000 | 93.97 |
| ATOM | 1426 | NE2 | HIS | A | 198 | -1.788  | -5.411 | 16.199 | 1.000 | 94.98 |
| ATOM | 1427 | CD2 | HIS | A | 198 | -1.280  | -4.259 | 16.747 | 1.000 | 92.03 |
| ATOM | 1428 | C   | HIS | A | 198 | -1.534  | -1.404 | 18.383 | 1.000 | 71.60 |
| ATOM | 1429 | O   | HIS | A | 198 | -2.374  | -1.488 | 17.480 | 1.000 | 79.54 |
| ATOM | 1430 | N   | ARG | A | 199 | -0.649  | -0.416 | 18.408 | 1.000 | 59.29 |
| ATOM | 1431 | CA  | ARG | A | 199 | -0.625  | 0.649  | 17.409 | 1.000 | 35.48 |
| ATOM | 1432 | CB  | ARG | A | 199 | -1.445  | 1.854  | 17.881 | 1.000 | 27.18 |
| ATOM | 1433 | CG  | ARG | A | 199 | -1.499  | 2.997  | 16.876 | 1.000 | 28.09 |
| ATOM | 1434 | CD  | ARG | A | 199 | -2.136  | 4.248  | 17.473 | 1.000 | 30.52 |
| ATOM | 1435 | NE  | ARG | A | 199 | -3.326  | 3.985  | 18.281 | 1.000 | 24.15 |
| ATOM | 1436 | CZ  | ARG | A | 199 | -3.802  | 4.809  | 19.209 | 1.000 | 28.77 |
| ATOM | 1437 | NH1 | ARG | A | 199 | -3.159  | 5.961  | 19.433 | 1.000 | 21.27 |
| ATOM | 1438 | NH2 | ARG | A | 199 | -4.894  | 4.481  | 19.891 | 1.000 | 20.72 |
| ATOM | 1439 | C   | ARG | A | 199 | 0.811   | 1.091  | 17.148 | 1.000 | 34.48 |
| ATOM | 1440 | O   | ARG | A | 199 | 1.652   | 1.004  | 18.041 | 1.000 | 33.43 |
| ATOM | 1441 | N   | LEU | A | 200 | 1.073   | 1.574  | 15.945 | 1.000 | 25.06 |
| ATOM | 1442 | CA  | LEU | A | 200 | 2.347   | 2.162  | 15.564 | 1.000 | 24.44 |
| ATOM | 1443 | CB  | LEU | A | 200 | 2.763   | 1.609  | 14.186 | 1.000 | 33.41 |
| ATOM | 1444 | CG  | LEU | A | 200 | 2.956   | 0.076  | 14.187 | 1.000 | 38.30 |
| ATOM | 1445 | CD1 | LEU | A | 200 | 3.183   | -0.457 | 12.783 | 1.000 | 34.53 |
| ATOM | 1446 | CD2 | LEU | A | 200 | 4.085   | -0.324 | 15.136 | 1.000 | 24.70 |
| ATOM | 1447 | C   | LEU | A | 200 | 2.247   | 3.680  | 15.530 | 1.000 | 27.60 |
| ATOM | 1448 | O   | LEU | A | 200 | 1.329   | 4.254  | 14.940 | 1.000 | 27.27 |
| ATOM | 1449 | N   | ILE | A | 201 | 3.190   | 4.352  | 16.167 | 1.000 | 21.65 |
| ATOM | 1450 | CA  | ILE | A | 201 | 3.223   | 5.805  | 16.195 | 1.000 | 19.45 |
| ATOM | 1451 | CB  | ILE | A | 201 | 3.243   | 6.350  | 17.634 | 1.000 | 23.93 |
| ATOM | 1452 | CG1 | ILE | A | 201 | 2.224   | 5.707  | 18.555 | 1.000 | 27.08 |
| ATOM | 1453 | CD1 | ILE | A | 201 | 0.840   | 6.267  | 18.547 | 1.000 | 32.15 |
| ATOM | 1454 | CG2 | ILE | A | 201 | 3.105   | 7.874  | 17.627 | 1.000 | 22.88 |
| ATOM | 1455 | C   | ILE | A | 201 | 4.494   | 6.275  | 15.498 | 1.000 | 16.73 |

**FIGURE 229**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1456 | O   | ILE | A | 201 | 5.543  | 5.697  | 15.797 | 1.000 | 21.43 |
| ATOM | 1457 | N   | ARG | A | 202 | 4.395  | 7.244  | 14.609 | 1.000 | 15.34 |
| ATOM | 1458 | CA  | ARG | A | 202 | 5.529  | 7.874  | 13.952 | 1.000 | 13.92 |
| ATOM | 1459 | CB  | ARG | A | 202 | 5.344  | 8.052  | 12.442 | 1.000 | 21.70 |
| ATOM | 1460 | CG  | ARG | A | 202 | 4.824  | 6.798  | 11.747 | 1.000 | 37.52 |
| ATOM | 1461 | CD  | ARG | A | 202 | 5.397  | 6.648  | 10.346 | 1.000 | 48.86 |
| ATOM | 1462 | NE  | ARG | A | 202 | 6.613  | 5.885  | 10.269 | 1.000 | 46.03 |
| ATOM | 1463 | CZ  | ARG | A | 202 | 7.751  | 6.058  | 9.632  | 1.000 | 45.70 |
| ATOM | 1464 | NH1 | ARG | A | 202 | 8.037  | 7.082  | 8.834  | 1.000 | 37.98 |
| ATOM | 1465 | NH2 | ARG | A | 202 | 8.673  | 5.112  | 9.812  | 1.000 | 32.36 |
| ATOM | 1466 | C   | ARG | A | 202 | 5.730  | 9.248  | 14.587 | 1.000 | 16.51 |
| ATOM | 1467 | O   | ARG | A | 202 | 4.762  | 9.959  | 14.863 | 1.000 | 18.08 |
| ATOM | 1468 | N   | HIS | A | 203 | 6.987  | 9.543  | 14.854 | 1.000 | 17.20 |
| ATOM | 1469 | CA  | HIS | A | 203 | 7.433  | 10.725 | 15.560 | 1.000 | 16.92 |
| ATOM | 1470 | CB  | HIS | A | 203 | 8.142  | 10.336 | 16.854 | 1.000 | 20.76 |
| ATOM | 1471 | CG  | HIS | A | 203 | 8.421  | 11.450 | 17.803 | 1.000 | 16.82 |
| ATOM | 1472 | ND1 | HIS | A | 203 | 9.626  | 12.125 | 17.837 | 1.000 | 21.78 |
| ATOM | 1473 | CE1 | HIS | A | 203 | 9.592  | 13.064 | 18.762 | 1.000 | 18.85 |
| ATOM | 1474 | NE2 | HIS | A | 203 | 8.404  | 13.021 | 19.331 | 1.000 | 19.59 |
| ATOM | 1475 | CD2 | HIS | A | 203 | 7.654  | 12.037 | 18.755 | 1.000 | 16.71 |
| ATOM | 1476 | C   | HIS | A | 203 | 8.357  | 11.516 | 14.629 | 1.000 | 15.29 |
| ATOM | 1477 | O   | HIS | A | 203 | 9.374  | 10.977 | 14.206 | 1.000 | 20.50 |
| ATOM | 1478 | N   | PHE | A | 204 | 7.949  | 12.737 | 14.315 | 1.000 | 19.40 |
| ATOM | 1479 | CA  | PHE | A | 204 | 8.668  | 13.627 | 13.398 | 1.000 | 22.59 |
| ATOM | 1480 | CB  | PHE | A | 204 | 7.750  | 14.112 | 12.280 | 1.000 | 16.25 |
| ATOM | 1481 | CG  | PHE | A | 204 | 7.133  | 12.949 | 11.535 | 1.000 | 19.17 |
| ATOM | 1482 | CD1 | PHE | A | 204 | 5.859  | 12.519 | 11.888 | 1.000 | 20.80 |
| ATOM | 1483 | CE1 | PHE | A | 204 | 5.296  | 11.466 | 11.195 | 1.000 | 18.80 |
| ATOM | 1484 | CZ  | PHE | A | 204 | 5.976  | 10.843 | 10.173 | 1.000 | 24.56 |
| ATOM | 1485 | CE2 | PHE | A | 204 | 7.246  | 11.266 | 9.820  | 1.000 | 23.53 |
| ATOM | 1486 | CD2 | PHE | A | 204 | 7.825  | 12.307 | 10.529 | 1.000 | 21.57 |
| ATOM | 1487 | C   | PHE | A | 204 | 9.237  | 14.789 | 14.191 | 1.000 | 15.29 |
| ATOM | 1488 | O   | PHE | A | 204 | 8.545  | 15.706 | 14.632 | 1.000 | 18.02 |
| ATOM | 1489 | N   | HIS | A | 205 | 10.552 | 14.693 | 14.407 | 1.000 | 17.57 |
| ATOM | 1490 | CA  | HIS | A | 205 | 11.231 | 15.586 | 15.336 | 1.000 | 20.77 |
| ATOM | 1491 | CB  | HIS | A | 205 | 12.017 | 14.705 | 16.297 | 1.000 | 22.15 |
| ATOM | 1492 | CG  | HIS | A | 205 | 12.733 | 15.407 | 17.404 | 1.000 | 23.38 |
| ATOM | 1493 | ND1 | HIS | A | 205 | 12.618 | 16.749 | 17.686 | 1.000 | 28.56 |
| ATOM | 1494 | CE1 | HIS | A | 205 | 13.372 | 17.053 | 18.726 | 1.000 | 22.17 |
| ATOM | 1495 | NE2 | HIS | A | 205 | 13.982 | 15.963 | 19.129 | 1.000 | 23.37 |
| ATOM | 1496 | CD2 | HIS | A | 205 | 13.598 | 14.913 | 18.326 | 1.000 | 19.72 |
| ATOM | 1497 | C   | HIS | A | 205 | 12.140 | 16.556 | 14.583 | 1.000 | 20.64 |
| ATOM | 1498 | O   | HIS | A | 205 | 13.207 | 16.157 | 14.120 | 1.000 | 20.31 |
| ATOM | 1499 | N   | TYR | A | 206 | 11.736 | 17.808 | 14.448 | 1.000 | 20.99 |
| ATOM | 1500 | CA  | TYR | A | 206 | 12.552 | 18.816 | 13.771 | 1.000 | 18.48 |
| ATOM | 1501 | CB  | TYR | A | 206 | 11.683 | 19.944 | 13.305 | 1.000 | 21.09 |
| ATOM | 1502 | CG  | TYR | A | 206 | 12.270 | 20.944 | 12.340 | 1.000 | 17.56 |
| ATOM | 1503 | CD1 | TYR | A | 206 | 12.517 | 20.592 | 11.011 | 1.000 | 16.37 |
| ATOM | 1504 | CE1 | TYR | A | 206 | 13.048 | 21.568 | 10.167 | 1.000 | 22.62 |
| ATOM | 1505 | CZ  | TYR | A | 206 | 13.294 | 22.833 | 10.665 | 1.000 | 23.75 |
| ATOM | 1506 | OH  | TYR | A | 206 | 13.820 | 23.786 | 9.833  | 1.000 | 24.85 |
| ATOM | 1507 | CE2 | TYR | A | 206 | 13.044 | 23.195 | 11.972 | 1.000 | 25.09 |

**FIGURE 230**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1508 | CD2 | TYR | A | 206 | 12.518 | 22.219 | 12.812 | 1.000 | 22.77 |
| ATOM | 1509 | C   | TYR | A | 206 | 13.580 | 19.341 | 14.783 | 1.000 | 16.12 |
| ATOM | 1510 | O   | TYR | A | 206 | 13.165 | 19.799 | 15.824 | 1.000 | 21.03 |
| ATOM | 1511 | N   | THR | A | 207 | 14.855 | 19.255 | 14.458 | 1.000 | 20.95 |
| ATOM | 1512 | CA  | THR | A | 207 | 15.937 | 19.446 | 15.406 | 1.000 | 25.39 |
| ATOM | 1513 | CB  | THR | A | 207 | 16.825 | 18.181 | 15.436 | 1.000 | 21.21 |
| ATOM | 1514 | OG1 | THR | A | 207 | 17.300 | 17.892 | 14.110 | 1.000 | 24.55 |
| ATOM | 1515 | CG2 | THR | A | 207 | 16.034 | 16.975 | 15.913 | 1.000 | 20.79 |
| ATOM | 1516 | C   | THR | A | 207 | 16.791 | 20.668 | 15.090 | 1.000 | 29.49 |
| ATOM | 1517 | O   | THR | A | 207 | 17.837 | 20.877 | 15.720 | 1.000 | 27.61 |
| ATOM | 1518 | N   | VAL | A | 208 | 16.366 | 21.501 | 14.140 | 1.000 | 24.45 |
| ATOM | 1519 | CA  | VAL | A | 208 | 17.216 | 22.662 | 13.859 | 1.000 | 21.06 |
| ATOM | 1520 | CB  | VAL | A | 208 | 17.883 | 22.496 | 12.481 | 1.000 | 28.39 |
| ATOM | 1521 | CG1 | VAL | A | 208 | 18.791 | 21.272 | 12.532 | 1.000 | 23.56 |
| ATOM | 1522 | CG2 | VAL | A | 208 | 16.849 | 22.387 | 11.368 | 1.000 | 20.57 |
| ATOM | 1523 | C   | VAL | A | 208 | 16.523 | 23.999 | 13.935 | 1.000 | 31.86 |
| ATOM | 1524 | O   | VAL | A | 208 | 17.084 | 24.981 | 13.417 | 1.000 | 27.99 |
| ATOM | 1525 | N   | TRP | A | 209 | 15.359 | 24.144 | 14.567 | 1.000 | 26.72 |
| ATOM | 1526 | CA  | TRP | A | 209 | 14.797 | 25.499 | 14.665 | 1.000 | 30.27 |
| ATOM | 1527 | CB  | TRP | A | 209 | 13.424 | 25.461 | 15.322 | 1.000 | 28.47 |
| ATOM | 1528 | CG  | TRP | A | 209 | 12.553 | 26.652 | 15.078 | 1.000 | 31.11 |
| ATOM | 1529 | CD1 | TRP | A | 209 | 12.747 | 27.933 | 15.523 | 1.000 | 31.15 |
| ATOM | 1530 | NE1 | TRP | A | 209 | 11.725 | 28.752 | 15.093 | 1.000 | 28.46 |
| ATOM | 1531 | CE2 | TRP | A | 209 | 10.845 | 28.000 | 14.356 | 1.000 | 28.45 |
| ATOM | 1532 | CD2 | TRP | A | 209 | 11.331 | 26.678 | 14.325 | 1.000 | 27.55 |
| ATOM | 1533 | CE3 | TRP | A | 209 | 10.611 | 25.704 | 13.629 | 1.000 | 22.81 |
| ATOM | 1534 | CZ3 | TRP | A | 209 | 9.445  | 26.095 | 13.005 | 1.000 | 25.86 |
| ATOM | 1535 | CH2 | TRP | A | 209 | 8.973  | 27.410 | 13.044 | 1.000 | 21.32 |
| ATOM | 1536 | CZ2 | TRP | A | 209 | 9.666  | 28.388 | 13.720 | 1.000 | 25.69 |
| ATOM | 1537 | C   | TRP | A | 209 | 15.756 | 26.384 | 15.452 | 1.000 | 27.61 |
| ATOM | 1538 | O   | TRP | A | 209 | 16.199 | 25.947 | 16.515 | 1.000 | 25.68 |
| ATOM | 1539 | N   | PRO | A | 210 | 16.119 | 27.575 | 15.000 | 1.000 | 24.36 |
| ATOM | 1540 | CA  | PRO | A | 210 | 17.083 | 28.369 | 15.787 | 1.000 | 26.72 |
| ATOM | 1541 | CB  | PRO | A | 210 | 17.398 | 29.537 | 14.854 | 1.000 | 23.52 |
| ATOM | 1542 | CG  | PRO | A | 210 | 16.330 | 29.568 | 13.828 | 1.000 | 30.83 |
| ATOM | 1543 | CD  | PRO | A | 210 | 15.721 | 28.197 | 13.735 | 1.000 | 24.56 |
| ATOM | 1544 | C   | PRO | A | 210 | 16.551 | 28.877 | 17.112 | 1.000 | 29.12 |
| ATOM | 1545 | O   | PRO | A | 210 | 15.359 | 29.056 | 17.335 | 1.000 | 26.48 |
| ATOM | 1546 | N   | ASP | A | 211 | 17.443 | 29.158 | 18.079 | 1.000 | 39.44 |
| ATOM | 1547 | CA  | ASP | A | 211 | 17.006 | 29.720 | 19.366 | 1.000 | 34.21 |
| ATOM | 1548 | CB  | ASP | A | 211 | 18.098 | 29.809 | 20.429 | 1.000 | 42.94 |
| ATOM | 1549 | CG  | ASP | A | 211 | 19.528 | 29.592 | 20.007 | 1.000 | 62.84 |
| ATOM | 1550 | OD1 | ASP | A | 211 | 20.028 | 30.231 | 19.044 | 1.000 | 74.38 |
| ATOM | 1551 | OD2 | ASP | A | 211 | 20.212 | 28.773 | 20.663 | 1.000 | 76.33 |
| ATOM | 1552 | C   | ASP | A | 211 | 16.433 | 31.124 | 19.187 | 1.000 | 35.17 |
| ATOM | 1553 | O   | ASP | A | 211 | 15.656 | 31.640 | 19.987 | 1.000 | 38.20 |
| ATOM | 1554 | N   | HIS | A | 212 | 16.818 | 31.816 | 18.113 | 1.000 | 39.51 |
| ATOM | 1555 | CA  | HIS | A | 212 | 16.184 | 33.125 | 17.909 | 1.000 | 42.28 |
| ATOM | 1556 | CB  | HIS | A | 212 | 17.197 | 34.250 | 18.143 | 1.000 | 51.96 |
| ATOM | 1557 | CG  | HIS | A | 212 | 17.690 | 34.249 | 19.563 | 1.000 | 70.14 |
| ATOM | 1558 | ND1 | HIS | A | 212 | 18.969 | 33.878 | 19.916 | 1.000 | 72.27 |
| ATOM | 1559 | CE1 | HIS | A | 212 | 19.109 | 33.968 | 21.227 | 1.000 | 71.31 |

**FIGURE 231**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1560 | NE2 | HIS | A | 212 | 17.962 | 34.385 | 21.735 | 1.000 | 73.22 |
| ATOM | 1561 | CD2 | HIS | A | 212 | 17.056 | 34.563 | 20.718 | 1.000 | 71.91 |
| ATOM | 1562 | C   | HIS | A | 212 | 15.568 | 33.188 | 16.521 | 1.000 | 35.23 |
| ATOM | 1563 | O   | HIS | A | 212 | 16.155 | 32.711 | 15.551 | 1.000 | 36.51 |
| ATOM | 1564 | N   | GLY | A | 213 | 14.380 | 33.777 | 16.425 | 1.000 | 39.89 |
| ATOM | 1565 | CA  | GLY | A | 213 | 13.712 | 33.934 | 15.149 | 1.000 | 35.59 |
| ATOM | 1566 | C   | GLY | A | 213 | 13.306 | 32.607 | 14.530 | 1.000 | 40.76 |
| ATOM | 1567 | O   | GLY | A | 213 | 13.230 | 31.604 | 15.240 | 1.000 | 29.83 |
| ATOM | 1568 | N   | VAL | A | 214 | 13.073 | 32.661 | 13.224 | 1.000 | 26.99 |
| ATOM | 1569 | CA  | VAL | A | 214 | 12.556 | 31.542 | 12.457 | 1.000 | 23.88 |
| ATOM | 1570 | CB  | VAL | A | 214 | 11.489 | 32.069 | 11.477 | 1.000 | 27.24 |
| ATOM | 1571 | CG1 | VAL | A | 214 | 10.282 | 32.612 | 12.225 | 1.000 | 25.46 |
| ATOM | 1572 | CG2 | VAL | A | 214 | 12.081 | 33.158 | 10.585 | 1.000 | 32.07 |
| ATOM | 1573 | C   | VAL | A | 214 | 13.672 | 30.841 | 11.701 | 1.000 | 33.49 |
| ATOM | 1574 | O   | VAL | A | 214 | 14.782 | 31.393 | 11.653 | 1.000 | 41.50 |
| ATOM | 1575 | N   | PRO | A | 215 | 13.433 | 29.666 | 11.132 | 1.000 | 33.79 |
| ATOM | 1576 | CA  | PRO | A | 215 | 14.416 | 29.011 | 10.262 | 1.000 | 32.45 |
| ATOM | 1577 | CB  | PRO | A | 215 | 13.625 | 27.863 | 9.628  | 1.000 | 27.07 |
| ATOM | 1578 | CG  | PRO | A | 215 | 12.646 | 27.518 | 10.693 | 1.000 | 25.47 |
| ATOM | 1579 | CD  | PRO | A | 215 | 12.228 | 28.835 | 11.297 | 1.000 | 29.25 |
| ATOM | 1580 | C   | PRO | A | 215 | 14.948 | 29.950 | 9.185  | 1.000 | 39.16 |
| ATOM | 1581 | O   | PRO | A | 215 | 14.249 | 30.839 | 8.704  | 1.000 | 42.31 |
| ATOM | 1582 | N   | GLU | A | 216 | 16.215 | 29.755 | 8.813  | 1.000 | 33.87 |
| ATOM | 1583 | CA  | GLU | A | 216 | 16.877 | 30.778 | 8.004  | 1.000 | 44.43 |
| ATOM | 1584 | CB  | GLU | A | 216 | 18.392 | 30.715 | 8.244  | 1.000 | 52.43 |
| ATOM | 1585 | CG  | GLU | A | 216 | 18.841 | 31.700 | 9.324  | 1.000 | 56.31 |
| ATOM | 1586 | CD  | GLU | A | 216 | 20.119 | 32.423 | 8.940  | 1.000 | 68.80 |
| ATOM | 1587 | OE1 | GLU | A | 216 | 20.015 | 33.454 | 8.242  | 1.000 | 80.56 |
| ATOM | 1588 | OE2 | GLU | A | 216 | 21.208 | 31.946 | 9.333  | 1.000 | 68.46 |
| ATOM | 1589 | C   | GLU | A | 216 | 16.531 | 30.688 | 6.522  | 1.000 | 40.23 |
| ATOM | 1590 | O   | GLU | A | 216 | 16.633 | 31.700 | 5.823  | 1.000 | 37.48 |
| ATOM | 1591 | N   | THR | A | 217 | 16.112 | 29.522 | 6.063  | 1.000 | 29.61 |
| ATOM | 1592 | CA  | THR | A | 217 | 15.492 | 29.314 | 4.778  | 1.000 | 32.71 |
| ATOM | 1593 | CB  | THR | A | 217 | 16.185 | 28.187 | 3.991  | 1.000 | 30.46 |
| ATOM | 1594 | OG1 | THR | A | 217 | 16.030 | 26.987 | 4.770  | 1.000 | 35.61 |
| ATOM | 1595 | CG2 | THR | A | 217 | 17.669 | 28.469 | 3.835  | 1.000 | 34.53 |
| ATOM | 1596 | C   | THR | A | 217 | 14.031 | 28.881 | 4.915  | 1.000 | 36.27 |
| ATOM | 1597 | O   | THR | A | 217 | 13.686 | 28.153 | 5.839  | 1.000 | 30.65 |
| ATOM | 1598 | N   | THR | A | 218 | 13.176 | 29.290 | 3.990  | 1.000 | 31.97 |
| ATOM | 1599 | CA  | THR | A | 218 | 11.842 | 28.692 | 3.901  | 1.000 | 22.66 |
| ATOM | 1600 | CB  | THR | A | 218 | 10.987 | 29.433 | 2.861  | 1.000 | 20.62 |
| ATOM | 1601 | OG1 | THR | A | 218 | 11.671 | 29.423 | 1.600  | 1.000 | 24.39 |
| ATOM | 1602 | CG2 | THR | A | 218 | 10.804 | 30.879 | 3.294  | 1.000 | 23.42 |
| ATOM | 1603 | C   | THR | A | 218 | 11.951 | 27.225 | 3.518  | 1.000 | 28.74 |
| ATOM | 1604 | O   | THR | A | 218 | 11.142 | 26.377 | 3.905  | 1.000 | 32.65 |
| ATOM | 1605 | N   | GLN | A | 219 | 12.969 | 26.889 | 2.721  | 1.000 | 25.74 |
| ATOM | 1606 | CA  | GLN | A | 219 | 13.056 | 25.550 | 2.173  | 1.000 | 20.41 |
| ATOM | 1607 | CB  | GLN | A | 219 | 14.365 | 25.386 | 1.388  | 1.000 | 28.06 |
| ATOM | 1608 | CG  | GLN | A | 219 | 14.167 | 24.541 | 0.137  | 1.000 | 47.72 |
| ATOM | 1609 | CD  | GLN | A | 219 | 14.872 | 23.201 | 0.253  | 1.000 | 57.11 |
| ATOM | 1610 | OE1 | GLN | A | 219 | 14.297 | 22.182 | -0.133 | 1.000 | 42.74 |
| ATOM | 1611 | NE2 | GLN | A | 219 | 16.096 | 23.246 | 0.779  | 1.000 | 56.71 |

**FIGURE 232**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1612 | C   | GLN | A | 219 | 13.010 | 24.421 | 3.211  | 1.000 | 22.65 |
| ATOM | 1613 | O   | GLN | A | 219 | 12.351 | 23.416 | 3.001  | 1.000 | 26.69 |
| ATOM | 1614 | N   | SER | A | 220 | 13.741 | 24.594 | 4.294  | 1.000 | 26.94 |
| ATOM | 1615 | CA  | SER | A | 220 | 13.846 | 23.658 | 5.400  | 1.000 | 30.86 |
| ATOM | 1616 | CB  | SER | A | 220 | 14.660 | 24.279 | 6.537  | 1.000 | 29.59 |
| ATOM | 1617 | OG  | SER | A | 220 | 14.662 | 23.505 | 7.717  | 1.000 | 28.43 |
| ATOM | 1618 | C   | SER | A | 220 | 12.463 | 23.280 | 5.946  | 1.000 | 20.04 |
| ATOM | 1619 | O   | SER | A | 220 | 12.135 | 22.096 | 5.958  | 1.000 | 27.37 |
| ATOM | 1620 | N   | LEU | A | 221 | 11.711 | 24.297 | 6.378  | 1.000 | 21.52 |
| ATOM | 1621 | CA  | LEU | A | 221 | 10.414 | 23.978 | 6.996  | 1.000 | 19.60 |
| ATOM | 1622 | CB  | LEU | A | 221 | 9.875  | 25.107 | 7.874  | 1.000 | 18.57 |
| ATOM | 1623 | CG  | LEU | A | 221 | 8.762  | 24.639 | 8.827  | 1.000 | 20.88 |
| ATOM | 1624 | CD1 | LEU | A | 221 | 9.333  | 23.645 | 9.830  | 1.000 | 24.60 |
| ATOM | 1625 | CD2 | LEU | A | 221 | 8.061  | 25.779 | 9.537  | 1.000 | 16.09 |
| ATOM | 1626 | C   | LEU | A | 221 | 9.436  | 23.546 | 5.914  | 1.000 | 21.46 |
| ATOM | 1627 | O   | LEU | A | 221 | 8.613  | 22.659 | 6.182  | 1.000 | 22.12 |
| ATOM | 1628 | N   | ILE | A | 222 | 9.507  | 24.112 | 4.703  | 1.000 | 21.43 |
| ATOM | 1629 | CA  | ILE | A | 222 | 8.594  | 23.627 | 3.661  | 1.000 | 19.51 |
| ATOM | 1630 | CB  | ILE | A | 222 | 8.782  | 24.425 | 2.352  | 1.000 | 17.06 |
| ATOM | 1631 | CG1 | ILE | A | 222 | 8.267  | 25.866 | 2.483  | 1.000 | 22.29 |
| ATOM | 1632 | CD1 | ILE | A | 222 | 8.545  | 26.686 | 1.227  | 1.000 | 25.18 |
| ATOM | 1633 | CG2 | ILE | A | 222 | 8.150  | 23.690 | 1.193  | 1.000 | 22.06 |
| ATOM | 1634 | C   | ILE | A | 222 | 8.788  | 22.150 | 3.399  | 1.000 | 23.90 |
| ATOM | 1635 | O   | ILE | A | 222 | 7.832  | 21.361 | 3.253  | 1.000 | 19.79 |
| ATOM | 1636 | N   | GLN | A | 223 | 10.049 | 21.706 | 3.348  | 1.000 | 23.36 |
| ATOM | 1637 | CA  | GLN | A | 223 | 10.361 | 20.297 | 3.096  | 1.000 | 22.31 |
| ATOM | 1638 | CB  | GLN | A | 223 | 11.867 | 20.094 | 2.866  | 1.000 | 27.99 |
| ATOM | 1639 | CG  | GLN | A | 223 | 12.297 | 18.683 | 2.510  | 1.000 | 27.69 |
| ATOM | 1640 | CD  | GLN | A | 223 | 11.727 | 18.170 | 1.203  | 1.000 | 36.04 |
| ATOM | 1641 | OE1 | GLN | A | 223 | 11.311 | 18.929 | 0.325  | 1.000 | 38.77 |
| ATOM | 1642 | NE2 | GLN | A | 223 | 11.677 | 16.854 | 1.025  | 1.000 | 34.81 |
| ATOM | 1643 | C   | GLN | A | 223 | 9.921  | 19.383 | 4.245  | 1.000 | 22.46 |
| ATOM | 1644 | O   | GLN | A | 223 | 9.447  | 18.263 | 3.994  | 1.000 | 19.87 |
| ATOM | 1645 | N   | PHE | A | 224 | 10.087 | 19.878 | 5.470  | 1.000 | 20.95 |
| ATOM | 1646 | CA  | PHE | A | 224 | 9.694  | 19.074 | 6.635  | 1.000 | 20.11 |
| ATOM | 1647 | CB  | PHE | A | 224 | 10.163 | 19.747 | 7.918  | 1.000 | 18.59 |
| ATOM | 1648 | CG  | PHE | A | 224 | 9.767  | 19.057 | 9.228  | 1.000 | 14.91 |
| ATOM | 1649 | CD1 | PHE | A | 224 | 10.211 | 17.795 | 9.547  | 1.000 | 18.83 |
| ATOM | 1650 | CE1 | PHE | A | 224 | 9.852  | 17.187 | 10.760 | 1.000 | 16.08 |
| ATOM | 1651 | CZ  | PHE | A | 224 | 9.030  | 17.866 | 11.638 | 1.000 | 14.76 |
| ATOM | 1652 | CE2 | PHE | A | 224 | 8.568  | 19.140 | 11.351 | 1.000 | 18.06 |
| ATOM | 1653 | CD2 | PHE | A | 224 | 8.947  | 19.716 | 10.141 | 1.000 | 19.42 |
| ATOM | 1654 | C   | PHE | A | 224 | 8.172  | 18.890 | 6.630  | 1.000 | 16.39 |
| ATOM | 1655 | O   | PHE | A | 224 | 7.689  | 17.764 | 6.787  | 1.000 | 18.08 |
| ATOM | 1656 | N   | VAL | A | 225 | 7.464  | 20.012 | 6.459  | 1.000 | 20.25 |
| ATOM | 1657 | CA  | VAL | A | 225 | 5.992  | 19.996 | 6.408  | 1.000 | 17.55 |
| ATOM | 1658 | CB  | VAL | A | 225 | 5.419  | 21.411 | 6.253  | 1.000 | 21.00 |
| ATOM | 1659 | CG1 | VAL | A | 225 | 3.947  | 21.344 | 5.850  | 1.000 | 16.31 |
| ATOM | 1660 | CG2 | VAL | A | 225 | 5.626  | 22.177 | 7.560  | 1.000 | 13.40 |
| ATOM | 1661 | C   | VAL | A | 225 | 5.512  | 19.084 | 5.298  | 1.000 | 17.64 |
| ATOM | 1662 | O   | VAL | A | 225 | 4.671  | 18.200 | 5.484  | 1.000 | 18.82 |
| ATOM | 1663 | N   | ARG | A | 226 | 6.062  | 19.192 | 4.088  | 1.000 | 19.58 |

**FIGURE 233**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1664 | CA  | ARG | A | 226 | 5.619  | 18.308 | 3.009  | 1.000 | 20.05 |
| ATOM | 1665 | CB  | ARG | A | 226 | 6.285  | 18.775 | 1.705  | 1.000 | 20.92 |
| ATOM | 1666 | CG  | ARG | A | 226 | 5.686  | 20.090 | 1.204  | 1.000 | 21.90 |
| ATOM | 1667 | CD  | ARG | A | 226 | 6.324  | 20.446 | -0.145 | 1.000 | 22.66 |
| ATOM | 1668 | NE  | ARG | A | 226 | 5.564  | 21.504 | -0.798 | 1.000 | 24.99 |
| ATOM | 1669 | CZ  | ARG | A | 226 | 6.095  | 22.322 | -1.697 | 1.000 | 40.94 |
| ATOM | 1670 | NH1 | ARG | A | 226 | 7.381  | 22.153 | -1.994 | 1.000 | 28.79 |
| ATOM | 1671 | NH2 | ARG | A | 226 | 5.371  | 23.272 | -2.281 | 1.000 | 30.57 |
| ATOM | 1672 | C   | ARG | A | 226 | 5.923  | 16.848 | 3.263  | 1.000 | 17.75 |
| ATOM | 1673 | O   | ARG | A | 226 | 5.172  | 15.933 | 2.955  | 1.000 | 19.58 |
| ATOM | 1674 | N   | THR | A | 227 | 7.055  | 16.531 | 3.881  | 1.000 | 19.90 |
| ATOM | 1675 | CA  | THR | A | 227 | 7.391  | 15.168 | 4.247  | 1.000 | 15.51 |
| ATOM | 1676 | CB  | THR | A | 227 | 8.835  | 15.143 | 4.821  | 1.000 | 21.32 |
| ATOM | 1677 | OG1 | THR | A | 227 | 9.764  | 15.609 | 3.823  | 1.000 | 22.05 |
| ATOM | 1678 | CG2 | THR | A | 227 | 9.217  | 13.723 | 5.189  | 1.000 | 20.98 |
| ATOM | 1679 | C   | THR | A | 227 | 6.413  | 14.588 | 5.271  | 1.000 | 15.49 |
| ATOM | 1680 | O   | THR | A | 227 | 5.919  | 13.477 | 5.141  | 1.000 | 19.20 |
| ATOM | 1681 | N   | VAL | A | 228 | 6.109  | 15.318 | 6.325  | 1.000 | 16.11 |
| ATOM | 1682 | CA  | VAL | A | 228 | 5.143  | 14.927 | 7.341  | 1.000 | 18.46 |
| ATOM | 1683 | CB  | VAL | A | 228 | 5.031  | 15.957 | 8.477  | 1.000 | 17.87 |
| ATOM | 1684 | CG1 | VAL | A | 228 | 3.887  | 15.568 | 9.414  | 1.000 | 18.37 |
| ATOM | 1685 | CG2 | VAL | A | 228 | 6.318  | 16.108 | 9.270  | 1.000 | 27.25 |
| ATOM | 1686 | C   | VAL | A | 228 | 3.751  | 14.744 | 6.713  | 1.000 | 17.43 |
| ATOM | 1687 | O   | VAL | A | 228 | 3.112  | 13.723 | 6.983  | 1.000 | 17.33 |
| ATOM | 1688 | N   | ARG | A | 229 | 3.338  | 15.721 | 5.898  | 1.000 | 18.35 |
| ATOM | 1689 | CA  | ARG | A | 229 | 2.003  | 15.683 | 5.292  | 1.000 | 20.21 |
| ATOM | 1690 | CB  | ARG | A | 229 | 1.710  | 16.982 | 4.560  | 1.000 | 20.48 |
| ATOM | 1691 | CG  | ARG | A | 229 | 0.475  | 16.989 | 3.670  | 1.000 | 22.85 |
| ATOM | 1692 | CD  | ARG | A | 229 | -0.750 | 16.409 | 4.384  | 1.000 | 19.41 |
| ATOM | 1693 | NE  | ARG | A | 229 | -1.031 | 17.165 | 5.615  | 1.000 | 19.35 |
| ATOM | 1694 | CZ  | ARG | A | 229 | -2.026 | 16.831 | 6.444  | 1.000 | 19.18 |
| ATOM | 1695 | NH1 | ARG | A | 229 | -2.773 | 15.784 | 6.097  | 1.000 | 19.75 |
| ATOM | 1696 | NH2 | ARG | A | 229 | -2.266 | 17.508 | 7.550  | 1.000 | 14.67 |
| ATOM | 1697 | C   | ARG | A | 229 | 1.917  | 14.434 | 4.421  | 1.000 | 25.70 |
| ATOM | 1698 | O   | ARG | A | 229 | 0.933  | 13.683 | 4.482  | 1.000 | 28.00 |
| ATOM | 1699 | N   | ASP | A | 230 | 2.949  | 14.152 | 3.627  | 1.000 | 23.44 |
| ATOM | 1700 | CA  | ASP | A | 230 | 3.008  | 12.884 | 2.886  | 1.000 | 26.19 |
| ATOM | 1701 | CB  | ASP | A | 230 | 4.322  | 12.757 | 2.098  | 1.000 | 25.54 |
| ATOM | 1702 | CG  | ASP | A | 230 | 4.325  | 13.611 | 0.845  | 1.000 | 39.61 |
| ATOM | 1703 | OD1 | ASP | A | 230 | 3.251  | 14.111 | 0.450  | 1.000 | 29.77 |
| ATOM | 1704 | OD2 | ASP | A | 230 | 5.398  | 13.806 | 0.233  | 1.000 | 42.44 |
| ATOM | 1705 | C   | ASP | A | 230 | 2.880  | 11.659 | 3.771  | 1.000 | 30.77 |
| ATOM | 1706 | O   | ASP | A | 230 | 2.146  | 10.713 | 3.455  | 1.000 | 27.25 |
| ATOM | 1707 | N   | TYR | A | 231 | 3.596  | 11.597 | 4.906  | 1.000 | 26.11 |
| ATOM | 1708 | CA  | TYR | A | 231 | 3.418  | 10.399 | 5.737  | 1.000 | 21.69 |
| ATOM | 1709 | CB  | TYR | A | 231 | 4.351  | 10.385 | 6.946  | 1.000 | 30.21 |
| ATOM | 1710 | CG  | TYR | A | 231 | 5.747  | 9.892  | 6.649  | 1.000 | 33.51 |
| ATOM | 1711 | CD1 | TYR | A | 231 | 5.992  | 8.543  | 6.409  | 1.000 | 34.93 |
| ATOM | 1712 | CE1 | TYR | A | 231 | 7.275  | 8.109  | 6.131  | 1.000 | 37.60 |
| ATOM | 1713 | CZ  | TYR | A | 231 | 8.331  | 8.999  | 6.092  | 1.000 | 28.01 |
| ATOM | 1714 | OH  | TYR | A | 231 | 9.604  | 8.546  | 5.820  | 1.000 | 29.93 |
| ATOM | 1715 | CE2 | TYR | A | 231 | 8.100  | 10.334 | 6.323  | 1.000 | 19.51 |

**FIGURE 234**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1716 | CD2 | TYR | A | 231 | 6.819  | 10.771 | 6.592  | 1.000 | 19.51 |
| ATOM | 1717 | C   | TYR | A | 231 | 1.994  | 10.314 | 6.274  | 1.000 | 26.15 |
| ATOM | 1718 | O   | TYR | A | 231 | 1.372  | 9.255  | 6.320  | 1.000 | 30.72 |
| ATOM | 1719 | N   | ILE | A | 232 | 1.503  | 11.467 | 6.729  | 1.000 | 22.90 |
| ATOM | 1720 | CA  | ILE | A | 232 | 0.167  | 11.452 | 7.319  | 1.000 | 24.42 |
| ATOM | 1721 | CB  | ILE | A | 232 | -0.271 | 12.843 | 7.788  | 1.000 | 28.90 |
| ATOM | 1722 | CG1 | ILE | A | 232 | 0.566  | 13.416 | 8.935  | 1.000 | 17.25 |
| ATOM | 1723 | CD1 | ILE | A | 232 | 0.205  | 14.859 | 9.204  | 1.000 | 22.29 |
| ATOM | 1724 | CG2 | ILE | A | 232 | -1.764 | 12.825 | 8.134  | 1.000 | 28.46 |
| ATOM | 1725 | C   | ILE | A | 232 | -0.881 | 10.941 | 6.329  | 1.000 | 26.86 |
| ATOM | 1726 | O   | ILE | A | 232 | -1.758 | 10.140 | 6.669  | 1.000 | 32.19 |
| ATOM | 1727 | N   | ASN | A | 233 | -0.764 | 11.429 | 5.106  | 1.000 | 25.93 |
| ATOM | 1728 | CA  | ASN | A | 233 | -1.751 | 11.166 | 4.070  | 1.000 | 30.21 |
| ATOM | 1729 | CB  | ASN | A | 233 | -1.549 | 12.124 | 2.900  | 1.000 | 24.13 |
| ATOM | 1730 | CG  | ASN | A | 233 | -2.266 | 13.446 | 3.088  | 1.000 | 31.27 |
| ATOM | 1731 | OD1 | ASN | A | 233 | -2.889 | 13.743 | 4.112  | 1.000 | 29.17 |
| ATOM | 1732 | ND2 | ASN | A | 233 | -2.134 | 14.239 | 2.035  | 1.000 | 30.92 |
| ATOM | 1733 | C   | ASN | A | 233 | -1.671 | 9.730  | 3.568  | 1.000 | 41.91 |
| ATOM | 1734 | O   | ASN | A | 233 | -2.603 | 9.199  | 2.958  | 1.000 | 41.91 |
| ATOM | 1735 | N   | ARG | A | 234 | -0.536 | 9.078  | 3.791  | 1.000 | 45.86 |
| ATOM | 1736 | CA  | ARG | A | 234 | -0.326 | 7.804  | 3.086  | 1.000 | 50.95 |
| ATOM | 1737 | CB  | ARG | A | 234 | 1.109  | 7.725  | 2.547  | 1.000 | 40.12 |
| ATOM | 1738 | CG  | ARG | A | 234 | 1.343  | 8.844  | 1.545  | 1.000 | 46.93 |
| ATOM | 1739 | CD  | ARG | A | 234 | 2.117  | 8.452  | 0.310  | 1.000 | 57.95 |
| ATOM | 1740 | NE  | ARG | A | 234 | 2.532  | 9.653  | -0.429 | 1.000 | 68.35 |
| ATOM | 1741 | CZ  | ARG | A | 234 | 3.780  | 10.094 | -0.506 | 1.000 | 67.12 |
| ATOM | 1742 | NH1 | ARG | A | 234 | 4.774  | 9.450  | 0.100  | 1.000 | 63.01 |
| ATOM | 1743 | NH2 | ARG | A | 234 | 4.041  | 11.192 | -1.199 | 1.000 | 61.94 |
| ATOM | 1744 | C   | ARG | A | 234 | -0.696 | 6.676  | 4.029  | 1.000 | 60.20 |
| ATOM | 1745 | O   | ARG | A | 234 | -0.601 | 5.491  | 3.730  | 1.000 | 87.41 |
| ATOM | 1746 | N   | SER | A | 235 | -1.146 | 7.142  | 5.194  | 1.000 | 44.81 |
| ATOM | 1747 | CA  | SER | A | 235 | -1.664 | 6.224  | 6.191  | 1.000 | 50.50 |
| ATOM | 1748 | CB  | SER | A | 235 | -1.332 | 6.720  | 7.596  | 1.000 | 40.08 |
| ATOM | 1749 | OG  | SER | A | 235 | -2.550 | 7.165  | 8.201  | 1.000 | 64.20 |
| ATOM | 1750 | C   | SER | A | 235 | -3.184 | 6.066  | 6.042  | 1.000 | 58.76 |
| ATOM | 1751 | O   | SER | A | 235 | -3.835 | 6.996  | 5.553  | 1.000 | 38.45 |
| ATOM | 1752 | N   | PRO | A | 236 | -3.665 | 4.905  | 6.477  | 1.000 | 62.13 |
| ATOM | 1753 | CA  | PRO | A | 236 | -5.059 | 4.491  | 6.327  | 1.000 | 58.65 |
| ATOM | 1754 | CB  | PRO | A | 236 | -5.065 | 3.010  | 6.716  | 1.000 | 53.85 |
| ATOM | 1755 | CG  | PRO | A | 236 | -3.634 | 2.599  | 6.792  | 1.000 | 49.45 |
| ATOM | 1756 | CD  | PRO | A | 236 | -2.898 | 3.851  | 7.185  | 1.000 | 58.01 |
| ATOM | 1757 | C   | PRO | A | 236 | -5.975 | 5.258  | 7.275  | 1.000 | 58.23 |
| ATOM | 1758 | O   | PRO | A | 236 | -7.033 | 5.742  | 6.887  | 1.000 | 62.93 |
| ATOM | 1759 | N   | GLY | A | 237 | -5.535 | 5.351  | 8.526  | 1.000 | 50.71 |
| ATOM | 1760 | CA  | GLY | A | 237 | -6.297 | 6.108  | 9.514  | 1.000 | 46.90 |
| ATOM | 1761 | C   | GLY | A | 237 | -5.292 | 6.580  | 10.552 | 1.000 | 55.40 |
| ATOM | 1762 | O   | GLY | A | 237 | -4.274 | 5.894  | 10.681 | 1.000 | 60.29 |
| ATOM | 1763 | N   | ALA | A | 238 | -5.566 | 7.689  | 11.229 | 1.000 | 61.94 |
| ATOM | 1764 | CA  | ALA | A | 238 | -4.552 | 8.203  | 12.150 | 1.000 | 56.95 |
| ATOM | 1765 | CB  | ALA | A | 238 | -3.434 | 8.854  | 11.328 | 1.000 | 52.44 |
| ATOM | 1766 | C   | ALA | A | 238 | -5.070 | 9.174  | 13.195 | 1.000 | 50.99 |
| ATOM | 1767 | O   | ALA | A | 238 | -4.242 | 9.571  | 14.033 | 1.000 | 57.56 |

**FIGURE 235**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1768 | N   | GLY | A | 239 | -6.349 | 9.552  | 13.199 | 1.000 | 34.51 |
| ATOM | 1769 | CA  | GLY | A | 239 | -6.845 | 10.375 | 14.310 | 1.000 | 33.83 |
| ATOM | 1770 | C   | GLY | A | 239 | -6.120 | 11.715 | 14.312 | 1.000 | 20.85 |
| ATOM | 1771 | O   | GLY | A | 239 | -5.394 | 11.963 | 13.335 | 1.000 | 30.52 |
| ATOM | 1772 | N   | PRO | A | 240 | -6.258 | 12.599 | 15.276 | 1.000 | 28.46 |
| ATOM | 1773 | CA  | PRO | A | 240 | -5.589 | 13.905 | 15.105 | 1.000 | 23.74 |
| ATOM | 1774 | CB  | PRO | A | 240 | -6.004 | 14.716 | 16.315 | 1.000 | 31.69 |
| ATOM | 1775 | CG  | PRO | A | 240 | -7.078 | 13.958 | 16.996 | 1.000 | 36.41 |
| ATOM | 1776 | CD  | PRO | A | 240 | -6.964 | 12.527 | 16.559 | 1.000 | 28.90 |
| ATOM | 1777 | C   | PRO | A | 240 | -4.072 | 13.702 | 15.099 | 1.000 | 25.52 |
| ATOM | 1778 | O   | PRO | A | 240 | -3.538 | 12.739 | 15.647 | 1.000 | 25.98 |
| ATOM | 1779 | N   | THR | A | 241 | -3.404 | 14.642 | 14.458 | 1.000 | 19.16 |
| ATOM | 1780 | CA  | THR | A | 241 | -1.954 | 14.695 | 14.504 | 1.000 | 17.79 |
| ATOM | 1781 | CB  | THR | A | 241 | -1.388 | 15.324 | 13.206 | 1.000 | 16.44 |
| ATOM | 1782 | OG1 | THR | A | 241 | -1.782 | 14.534 | 12.091 | 1.000 | 18.37 |
| ATOM | 1783 | CG2 | THR | A | 241 | 0.130  | 15.352 | 13.322 | 1.000 | 18.85 |
| ATOM | 1784 | C   | THR | A | 241 | -1.547 | 15.547 | 15.690 | 1.000 | 16.03 |
| ATOM | 1785 | O   | THR | A | 241 | -2.027 | 16.671 | 15.783 | 1.000 | 14.26 |
| ATOM | 1786 | N   | VAL | A | 242 | -0.710 | 15.081 | 16.604 | 1.000 | 14.89 |
| ATOM | 1787 | CA  | VAL | A | 242 | -0.276 | 15.964 | 17.707 | 1.000 | 12.20 |
| ATOM | 1788 | CB  | VAL | A | 242 | 0.120  | 15.076 | 18.909 | 1.000 | 15.21 |
| ATOM | 1789 | CG1 | VAL | A | 242 | 0.983  | 15.784 | 19.937 | 1.000 | 15.58 |
| ATOM | 1790 | CG2 | VAL | A | 242 | -1.132 | 14.525 | 19.592 | 1.000 | 15.20 |
| ATOM | 1791 | C   | VAL | A | 242 | 0.896  | 16.806 | 17.253 | 1.000 | 15.62 |
| ATOM | 1792 | O   | VAL | A | 242 | 1.838  | 16.295 | 16.614 | 1.000 | 16.25 |
| ATOM | 1793 | N   | VAL | A | 243 | 0.877  | 18.091 | 17.577 | 1.000 | 13.63 |
| ATOM | 1794 | CA  | VAL | A | 243 | 1.995  | 18.961 | 17.231 | 1.000 | 14.54 |
| ATOM | 1795 | CB  | VAL | A | 243 | 1.707  | 19.938 | 16.086 | 1.000 | 18.21 |
| ATOM | 1796 | CG1 | VAL | A | 243 | 2.970  | 20.692 | 15.648 | 1.000 | 15.88 |
| ATOM | 1797 | CG2 | VAL | A | 243 | 1.120  | 19.216 | 14.869 | 1.000 | 17.94 |
| ATOM | 1798 | C   | VAL | A | 243 | 2.377  | 19.709 | 18.502 | 1.000 | 14.26 |
| ATOM | 1799 | O   | VAL | A | 243 | 1.559  | 20.250 | 19.248 | 1.000 | 16.04 |
| ATOM | 1800 | N   | HIS | A | 244 | 3.686  | 19.752 | 18.781 | 1.000 | 17.37 |
| ATOM | 1801 | CA  | HIS | A | 244 | 4.097  | 20.519 | 19.951 | 1.000 | 14.10 |
| ATOM | 1802 | CB  | HIS | A | 244 | 4.022  | 19.648 | 21.202 | 1.000 | 15.84 |
| ATOM | 1803 | CG  | HIS | A | 244 | 5.142  | 18.657 | 21.367 | 1.000 | 17.02 |
| ATOM | 1804 | ND1 | HIS | A | 244 | 6.351  | 19.001 | 21.955 | 1.000 | 21.61 |
| ATOM | 1805 | CE1 | HIS | A | 244 | 7.130  | 17.936 | 21.988 | 1.000 | 17.38 |
| ATOM | 1806 | NE2 | HIS | A | 244 | 6.471  | 16.897 | 21.474 | 1.000 | 16.96 |
| ATOM | 1807 | CD2 | HIS | A | 244 | 5.226  | 17.346 | 21.099 | 1.000 | 12.72 |
| ATOM | 1808 | C   | HIS | A | 244 | 5.511  | 21.073 | 19.792 | 1.000 | 15.92 |
| ATOM | 1809 | O   | HIS | A | 244 | 6.302  | 20.556 | 18.999 | 1.000 | 15.50 |
| ATOM | 1810 | N   | CYS | A | 245 | 5.762  | 22.123 | 20.572 | 1.000 | 19.65 |
| ATOM | 1811 | CA  | CYS | A | 245 | 7.129  | 22.659 | 20.697 | 1.000 | 23.91 |
| ATOM | 1812 | CB  | CYS | A | 245 | 7.258  | 24.015 | 19.998 | 1.000 | 21.22 |
| ATOM | 1813 | SG  | CYS | A | 245 | 5.939  | 25.207 | 20.299 | 1.000 | 27.54 |
| ATOM | 1814 | C   | CYS | A | 245 | 7.436  | 22.703 | 22.181 | 1.000 | 25.09 |
| ATOM | 1815 | O   | CYS | A | 245 | 7.226  | 21.699 | 22.894 | 1.000 | 22.16 |
| ATOM | 1816 | N   | SER | A | 246 | 7.888  | 23.809 | 22.751 | 1.000 | 19.84 |
| ATOM | 1817 | CA  | SER | A | 246 | 7.969  | 23.838 | 24.223 | 1.000 | 16.95 |
| ATOM | 1818 | CB  | SER | A | 246 | 9.152  | 24.728 | 24.635 | 1.000 | 22.80 |
| ATOM | 1819 | OG  | SER | A | 246 | 9.277  | 24.846 | 26.034 | 1.000 | 23.37 |

**FIGURE 236**



|      |      |     |           |        |        |        |       |       |
|------|------|-----|-----------|--------|--------|--------|-------|-------|
| ATOM | 1820 | C   | SER A 246 | 6.660  | 24.303 | 24.834 | 1.000 | 18.58 |
| ATOM | 1821 | O   | SER A 246 | 6.097  | 23.705 | 25.756 | 1.000 | 23.44 |
| ATOM | 1822 | N   | ALA A 247 | 6.105  | 25.428 | 24.344 | 1.000 | 21.38 |
| ATOM | 1823 | CA  | ALA A 247 | 4.834  | 25.878 | 24.909 | 1.000 | 26.84 |
| ATOM | 1824 | CB  | ALA A 247 | 4.815  | 27.397 | 25.044 | 1.000 | 30.94 |
| ATOM | 1825 | C   | ALA A 247 | 3.627  | 25.429 | 24.082 | 1.000 | 18.61 |
| ATOM | 1826 | O   | ALA A 247 | 2.500  | 25.492 | 24.563 | 1.000 | 23.09 |
| ATOM | 1827 | N   | GLY A 248 | 3.876  | 24.984 | 22.867 | 1.000 | 20.85 |
| ATOM | 1828 | CA  | GLY A 248 | 2.846  | 24.579 | 21.933 | 1.000 | 24.45 |
| ATOM | 1829 | C   | GLY A 248 | 2.113  | 25.731 | 21.278 | 1.000 | 30.38 |
| ATOM | 1830 | O   | GLY A 248 | 0.928  | 25.550 | 20.948 | 1.000 | 32.96 |
| ATOM | 1831 | N   | VAL A 249 | 2.794  | 26.852 | 21.091 | 1.000 | 21.75 |
| ATOM | 1832 | CA  | VAL A 249 | 2.214  | 28.061 | 20.510 | 1.000 | 26.90 |
| ATOM | 1833 | CB  | VAL A 249 | 2.293  | 29.257 | 21.504 | 1.000 | 35.49 |
| ATOM | 1834 | CG1 | VAL A 249 | 1.266  | 29.099 | 22.616 | 1.000 | 56.26 |
| ATOM | 1835 | CG2 | VAL A 249 | 3.654  | 29.410 | 22.145 | 1.000 | 24.47 |
| ATOM | 1836 | C   | VAL A 249 | 2.839  | 28.525 | 19.210 | 1.000 | 22.79 |
| ATOM | 1837 | O   | VAL A 249 | 2.200  | 28.508 | 18.151 | 1.000 | 26.47 |
| ATOM | 1838 | N   | GLY A 250 | 4.064  | 29.056 | 19.197 | 1.000 | 24.61 |
| ATOM | 1839 | CA  | GLY A 250 | 4.490  | 29.816 | 18.032 | 1.000 | 16.91 |
| ATOM | 1840 | C   | GLY A 250 | 4.953  | 28.914 | 16.917 | 1.000 | 21.72 |
| ATOM | 1841 | O   | GLY A 250 | 4.438  | 28.910 | 15.787 | 1.000 | 20.15 |
| ATOM | 1842 | N   | ARG A 251 | 5.967  | 28.114 | 17.253 | 1.000 | 19.78 |
| ATOM | 1843 | CA  | ARG A 251 | 6.512  | 27.182 | 16.284 | 1.000 | 21.28 |
| ATOM | 1844 | CB  | ARG A 251 | 7.717  | 26.381 | 16.767 | 1.000 | 26.04 |
| ATOM | 1845 | CG  | ARG A 251 | 8.878  | 27.181 | 17.346 | 1.000 | 34.41 |
| ATOM | 1846 | CD  | ARG A 251 | 10.132 | 26.322 | 17.479 | 1.000 | 26.22 |
| ATOM | 1847 | NE  | ARG A 251 | 11.199 | 27.043 | 18.161 | 1.000 | 30.53 |
| ATOM | 1848 | CZ  | ARG A 251 | 12.191 | 26.523 | 18.874 | 1.000 | 32.54 |
| ATOM | 1849 | NH1 | ARG A 251 | 12.297 | 25.212 | 19.033 | 1.000 | 22.98 |
| ATOM | 1850 | NH2 | ARG A 251 | 13.080 | 27.349 | 19.428 | 1.000 | 27.69 |
| ATOM | 1851 | C   | ARG A 251 | 5.417  | 26.194 | 15.829 | 1.000 | 22.23 |
| ATOM | 1852 | O   | ARG A 251 | 5.358  | 25.859 | 14.651 | 1.000 | 15.33 |
| ATOM | 1853 | N   | THR A 252 | 4.631  | 25.769 | 16.810 | 1.000 | 19.69 |
| ATOM | 1854 | CA  | THR A 252 | 3.579  | 24.773 | 16.547 | 1.000 | 20.16 |
| ATOM | 1855 | CB  | THR A 252 | 2.960  | 24.322 | 17.888 | 1.000 | 22.57 |
| ATOM | 1856 | OG1 | THR A 252 | 3.926  | 23.485 | 18.569 | 1.000 | 20.75 |
| ATOM | 1857 | CG2 | THR A 252 | 1.709  | 23.474 | 17.699 | 1.000 | 17.40 |
| ATOM | 1858 | C   | THR A 252 | 2.554  | 25.401 | 15.618 | 1.000 | 18.08 |
| ATOM | 1859 | O   | THR A 252 | 2.136  | 24.800 | 14.632 | 1.000 | 19.10 |
| ATOM | 1860 | N   | GLY A 253 | 2.134  | 26.639 | 15.924 | 1.000 | 17.29 |
| ATOM | 1861 | CA  | GLY A 253 | 1.142  | 27.297 | 15.074 | 1.000 | 14.74 |
| ATOM | 1862 | C   | GLY A 253 | 1.662  | 27.585 | 13.675 | 1.000 | 23.43 |
| ATOM | 1863 | O   | GLY A 253 | 0.946  | 27.483 | 12.672 | 1.000 | 14.99 |
| ATOM | 1864 | N   | THR A 254 | 2.940  | 27.949 | 13.575 | 1.000 | 18.08 |
| ATOM | 1865 | CA  | THR A 254 | 3.601  | 28.145 | 12.289 | 1.000 | 17.61 |
| ATOM | 1866 | CB  | THR A 254 | 5.014  | 28.741 | 12.533 | 1.000 | 16.64 |
| ATOM | 1867 | OG1 | THR A 254 | 4.873  | 29.982 | 13.251 | 1.000 | 20.15 |
| ATOM | 1868 | CG2 | THR A 254 | 5.694  | 29.043 | 11.221 | 1.000 | 17.02 |
| ATOM | 1869 | C   | THR A 254 | 3.643  | 26.845 | 11.511 | 1.000 | 16.81 |
| ATOM | 1870 | O   | THR A 254 | 3.355  | 26.769 | 10.313 | 1.000 | 17.03 |
| ATOM | 1871 | N   | PHE A 255 | 3.981  | 25.701 | 12.162 | 1.000 | 17.85 |

FIGURE 237

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|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1872 | CA  | PHE | A | 255 | 3.963  | 24.414 | 11.477 | 1.000 | 13.47 |
| ATOM | 1873 | CB  | PHE | A | 255 | 4.343  | 23.241 | 12.408 | 1.000 | 13.89 |
| ATOM | 1874 | CG  | PHE | A | 255 | 4.219  | 21.881 | 11.732 | 1.000 | 14.73 |
| ATOM | 1875 | CD1 | PHE | A | 255 | 5.240  | 21.372 | 10.954 | 1.000 | 12.62 |
| ATOM | 1876 | CE1 | PHE | A | 255 | 5.203  | 20.153 | 10.292 | 1.000 | 16.48 |
| ATOM | 1877 | CZ  | PHE | A | 255 | 4.042  | 19.390 | 10.390 | 1.000 | 17.68 |
| ATOM | 1878 | CE2 | PHE | A | 255 | 3.012  | 19.881 | 11.182 | 1.000 | 13.26 |
| ATOM | 1879 | CD2 | PHE | A | 255 | 3.081  | 21.074 | 11.855 | 1.000 | 16.37 |
| ATOM | 1880 | C   | PHE | A | 255 | 2.554  | 24.154 | 10.899 | 1.000 | 10.19 |
| ATOM | 1881 | O   | PHE | A | 255 | 2.385  | 23.771 | 9.748  | 1.000 | 15.90 |
| ATOM | 1882 | N   | ILE | A | 256 | 1.557  | 24.332 | 11.785 | 1.000 | 12.97 |
| ATOM | 1883 | CA  | ILE | A | 256 | 0.188  | 23.972 | 11.333 | 1.000 | 13.95 |
| ATOM | 1884 | CB  | ILE | A | 256 | -0.779 | 23.954 | 12.523 | 1.000 | 13.52 |
| ATOM | 1885 | CG1 | ILE | A | 256 | -0.475 | 22.759 | 13.451 | 1.000 | 15.18 |
| ATOM | 1886 | CD1 | ILE | A | 256 | -1.294 | 22.825 | 14.733 | 1.000 | 19.48 |
| ATOM | 1887 | CG2 | ILE | A | 256 | -2.238 | 23.941 | 12.124 | 1.000 | 19.86 |
| ATOM | 1888 | C   | ILE | A | 256 | -0.290 | 24.885 | 10.223 | 1.000 | 12.32 |
| ATOM | 1889 | O   | ILE | A | 256 | -0.822 | 24.432 | 9.205  | 1.000 | 16.82 |
| ATOM | 1890 | N   | ALA | A | 257 | -0.075 | 26.179 | 10.375 | 1.000 | 13.56 |
| ATOM | 1891 | CA  | ALA | A | 257 | -0.526 | 27.108 | 9.330  | 1.000 | 13.60 |
| ATOM | 1892 | CB  | ALA | A | 257 | -0.232 | 28.522 | 9.818  | 1.000 | 18.20 |
| ATOM | 1893 | C   | ALA | A | 257 | 0.148  | 26.789 | 8.011  | 1.000 | 17.01 |
| ATOM | 1894 | O   | ALA | A | 257 | -0.446 | 26.751 | 6.923  | 1.000 | 16.67 |
| ATOM | 1895 | N   | LEU | A | 258 | 1.461  | 26.519 | 8.059  | 1.000 | 17.25 |
| ATOM | 1896 | CA  | LEU | A | 258 | 2.147  | 26.158 | 6.822  | 1.000 | 17.53 |
| ATOM | 1897 | CB  | LEU | A | 258 | 3.654  | 26.013 | 7.044  | 1.000 | 17.08 |
| ATOM | 1898 | CG  | LEU | A | 258 | 4.507  | 25.868 | 5.780  | 1.000 | 20.80 |
| ATOM | 1899 | CD1 | LEU | A | 258 | 4.222  | 27.003 | 4.793  | 1.000 | 15.05 |
| ATOM | 1900 | CD2 | LEU | A | 258 | 5.992  | 25.859 | 6.121  | 1.000 | 18.82 |
| ATOM | 1901 | C   | LEU | A | 258 | 1.622  | 24.850 | 6.248  | 1.000 | 18.92 |
| ATOM | 1902 | O   | LEU | A | 258 | 1.448  | 24.706 | 5.036  | 1.000 | 18.97 |
| ATOM | 1903 | N   | ASP | A | 259 | 1.363  | 23.837 | 7.090  | 1.000 | 16.07 |
| ATOM | 1904 | CA  | ASP | A | 259 | 0.754  | 22.618 | 6.578  | 1.000 | 10.97 |
| ATOM | 1905 | CB  | ASP | A | 259 | 0.551  | 21.650 | 7.742  | 1.000 | 13.81 |
| ATOM | 1906 | CG  | ASP | A | 259 | -0.025 | 20.310 | 7.371  | 1.000 | 17.58 |
| ATOM | 1907 | OD1 | ASP | A | 259 | 0.282  | 19.727 | 6.307  | 1.000 | 16.06 |
| ATOM | 1908 | OD2 | ASP | A | 259 | -0.800 | 19.817 | 8.233  | 1.000 | 19.09 |
| ATOM | 1909 | C   | ASP | A | 259 | -0.574 | 22.893 | 5.858  | 1.000 | 13.42 |
| ATOM | 1910 | O   | ASP | A | 259 | -0.784 | 22.386 | 4.764  | 1.000 | 18.06 |
| ATOM | 1911 | N   | ARG | A | 260 | -1.456 | 23.673 | 6.457  | 1.000 | 15.30 |
| ATOM | 1912 | CA  | ARG | A | 260 | -2.741 | 24.034 | 5.845  | 1.000 | 17.67 |
| ATOM | 1913 | CB  | ARG | A | 260 | -3.567 | 24.849 | 6.842  | 1.000 | 14.27 |
| ATOM | 1914 | CG  | ARG | A | 260 | -3.970 | 24.009 | 8.067  | 1.000 | 12.81 |
| ATOM | 1915 | CD  | ARG | A | 260 | -4.923 | 24.884 | 8.885  | 1.000 | 20.83 |
| ATOM | 1916 | NE  | ARG | A | 260 | -6.158 | 25.124 | 8.125  | 1.000 | 27.40 |
| ATOM | 1917 | CZ  | ARG | A | 260 | -7.185 | 25.786 | 8.663  | 1.000 | 40.82 |
| ATOM | 1918 | NH1 | ARG | A | 260 | -7.082 | 26.236 | 9.907  | 1.000 | 36.06 |
| ATOM | 1919 | NH2 | ARG | A | 260 | -8.288 | 25.988 | 7.962  | 1.000 | 39.48 |
| ATOM | 1920 | C   | ARG | A | 260 | -2.523 | 24.808 | 4.549  | 1.000 | 19.93 |
| ATOM | 1921 | O   | ARG | A | 260 | -3.148 | 24.535 | 3.519  | 1.000 | 17.22 |
| ATOM | 1922 | N   | ILE | A | 261 | -1.618 | 25.791 | 4.553  | 1.000 | 16.11 |
| ATOM | 1923 | CA  | ILE | A | 261 | -1.516 | 26.628 | 3.338  | 1.000 | 17.32 |

**FIGURE 238**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 1924 | CB  | ILE | A | 261 | -0.841 | 27.994 | 3.615  | 1.000 | 21.93 |
| ATOM | 1925 | CG1 | ILE | A | 261 | 0.658  | 27.969 | 3.875  | 1.000 | 27.34 |
| ATOM | 1926 | CD1 | ILE | A | 261 | 1.186  | 29.227 | 4.546  | 1.000 | 33.86 |
| ATOM | 1927 | CG2 | ILE | A | 261 | -1.581 | 28.703 | 4.758  | 1.000 | 18.92 |
| ATOM | 1928 | C   | ILE | A | 261 | -0.851 | 25.876 | 2.216  | 1.000 | 20.48 |
| ATOM | 1929 | O   | ILE | A | 261 | -1.226 | 26.009 | 1.034  | 1.000 | 22.32 |
| ATOM | 1930 | N   | LEU | A | 262 | 0.143  | 25.028 | 2.509  | 1.000 | 16.93 |
| ATOM | 1931 | CA  | LEU | A | 262 | 0.737  | 24.302 | 1.387  | 1.000 | 17.22 |
| ATOM | 1932 | CB  | LEU | A | 262 | 1.975  | 23.501 | 1.820  | 1.000 | 16.74 |
| ATOM | 1933 | CG  | LEU | A | 262 | 3.194  | 24.340 | 2.240  | 1.000 | 20.68 |
| ATOM | 1934 | CD1 | LEU | A | 262 | 4.319  | 23.422 | 2.693  | 1.000 | 18.57 |
| ATOM | 1935 | CD2 | LEU | A | 262 | 3.634  | 25.246 | 1.085  | 1.000 | 18.30 |
| ATOM | 1936 | C   | LEU | A | 262 | -0.280 | 23.362 | 0.776  | 1.000 | 19.77 |
| ATOM | 1937 | O   | LEU | A | 262 | -0.261 | 23.155 | -0.436 | 1.000 | 20.56 |
| ATOM | 1938 | N   | GLN | A | 263 | -1.139 | 22.759 | 1.613  | 1.000 | 19.67 |
| ATOM | 1939 | CA  | GLN | A | 263 | -2.241 | 21.952 | 1.056  | 1.000 | 19.49 |
| ATOM | 1940 | CB  | GLN | A | 263 | -3.050 | 21.287 | 2.170  | 1.000 | 17.39 |
| ATOM | 1941 | CG  | GLN | A | 263 | -2.289 | 20.167 | 2.891  | 1.000 | 15.52 |
| ATOM | 1942 | CD  | GLN | A | 263 | -3.138 | 19.572 | 4.012  | 1.000 | 20.67 |
| ATOM | 1943 | OE1 | GLN | A | 263 | -3.928 | 18.638 | 3.850  | 1.000 | 20.81 |
| ATOM | 1944 | NE2 | GLN | A | 263 | -2.956 | 20.185 | 5.176  | 1.000 | 17.87 |
| ATOM | 1945 | C   | GLN | A | 263 | -3.138 | 22.833 | 0.183  | 1.000 | 13.70 |
| ATOM | 1946 | O   | GLN | A | 263 | -3.554 | 22.415 | -0.904 | 1.000 | 24.55 |
| ATOM | 1947 | N   | GLN | A | 264 | -3.444 | 24.043 | 0.641  | 1.000 | 15.00 |
| ATOM | 1948 | CA  | GLN | A | 264 | -4.260 | 24.907 | -0.217 | 1.000 | 22.95 |
| ATOM | 1949 | CB  | GLN | A | 264 | -4.553 | 26.223 | 0.485  | 1.000 | 26.53 |
| ATOM | 1950 | CG  | GLN | A | 264 | -5.586 | 26.136 | 1.595  | 1.000 | 29.68 |
| ATOM | 1951 | CD  | GLN | A | 264 | -5.638 | 27.472 | 2.328  | 1.000 | 32.15 |
| ATOM | 1952 | OE1 | GLN | A | 264 | -5.197 | 28.482 | 1.781  | 1.000 | 29.91 |
| ATOM | 1953 | NE2 | GLN | A | 264 | -6.154 | 27.458 | 3.550  | 1.000 | 38.37 |
| ATOM | 1954 | C   | GLN | A | 264 | -3.583 | 25.159 | -1.559 | 1.000 | 21.95 |
| ATOM | 1955 | O   | GLN | A | 264 | -4.225 | 25.050 | -2.610 | 1.000 | 24.60 |
| ATOM | 1956 | N   | LEU | A | 265 | -2.293 | 25.490 | -1.552 | 1.000 | 16.75 |
| ATOM | 1957 | CA  | LEU | A | 265 | -1.536 | 25.721 | -2.771 | 1.000 | 19.81 |
| ATOM | 1958 | CB  | LEU | A | 265 | -0.067 | 26.053 | -2.420 | 1.000 | 23.63 |
| ATOM | 1959 | CG  | LEU | A | 265 | 0.195  | 27.420 | -1.807 | 1.000 | 29.98 |
| ATOM | 1960 | CD1 | LEU | A | 265 | 1.682  | 27.725 | -1.734 | 1.000 | 26.97 |
| ATOM | 1961 | CD2 | LEU | A | 265 | -0.519 | 28.505 | -2.613 | 1.000 | 33.62 |
| ATOM | 1962 | C   | LEU | A | 265 | -1.541 | 24.553 | -3.735 | 1.000 | 19.01 |
| ATOM | 1963 | O   | LEU | A | 265 | -1.324 | 24.723 | -4.947 | 1.000 | 22.58 |
| ATOM | 1964 | N   | ASP | A | 266 | -1.767 | 23.324 | -3.273 | 1.000 | 19.07 |
| ATOM | 1965 | CA  | ASP | A | 266 | -1.801 | 22.167 | -4.139 | 1.000 | 16.52 |
| ATOM | 1966 | CB  | ASP | A | 266 | -1.173 | 20.917 | -3.509 | 1.000 | 22.85 |
| ATOM | 1967 | CG  | ASP | A | 266 | 0.336  | 21.022 | -3.334 | 1.000 | 25.04 |
| ATOM | 1968 | OD1 | ASP | A | 266 | 0.957  | 21.963 | -3.836 | 1.000 | 21.32 |
| ATOM | 1969 | OD2 | ASP | A | 266 | 0.899  | 20.138 | -2.658 | 1.000 | 26.79 |
| ATOM | 1970 | C   | ASP | A | 266 | -3.227 | 21.776 | -4.570 | 1.000 | 17.40 |
| ATOM | 1971 | O   | ASP | A | 266 | -3.354 | 20.825 | -5.337 | 1.000 | 24.62 |
| ATOM | 1972 | N   | SER | A | 267 | -4.231 | 22.487 | -4.092 | 1.000 | 22.55 |
| ATOM | 1973 | CA  | SER | A | 267 | -5.619 | 22.129 | -4.359 | 1.000 | 24.11 |
| ATOM | 1974 | CB  | SER | A | 267 | -6.289 | 21.776 | -3.019 | 1.000 | 23.25 |
| ATOM | 1975 | OG  | SER | A | 267 | -6.418 | 20.374 | -2.892 | 1.000 | 34.75 |

**FIGURE 239**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |           |         |        |        |       |       |
|------|------|-----|-----------|---------|--------|--------|-------|-------|
| ATOM | 1976 | C   | SER A 267 | -6.419  | 23.235 | -5.033 | 1.000 | 19.22 |
| ATOM | 1977 | O   | SER A 267 | -7.300  | 22.941 | -5.859 | 1.000 | 20.89 |
| ATOM | 1978 | N   | LYS A 268 | -6.137  | 24.463 | -4.684 | 1.000 | 21.22 |
| ATOM | 1979 | CA  | LYS A 268 | -6.907  | 25.624 | -5.091 | 1.000 | 30.13 |
| ATOM | 1980 | CB  | LYS A 268 | -7.595  | 26.250 | -3.869 | 1.000 | 24.53 |
| ATOM | 1981 | CG  | LYS A 268 | -8.563  | 25.304 | -3.175 | 1.000 | 30.56 |
| ATOM | 1982 | CD  | LYS A 268 | -8.969  | 25.910 | -1.838 | 1.000 | 28.63 |
| ATOM | 1983 | CE  | LYS A 268 | -10.158 | 26.834 | -1.992 | 1.000 | 29.96 |
| ATOM | 1984 | NZ  | LYS A 268 | -10.686 | 27.208 | -0.641 | 1.000 | 30.06 |
| ATOM | 1985 | C   | LYS A 268 | -6.095  | 26.737 | -5.735 | 1.000 | 30.67 |
| ATOM | 1986 | O   | LYS A 268 | -4.872  | 26.833 | -5.660 | 1.000 | 23.21 |
| ATOM | 1987 | N   | ASP A 269 | -6.834  | 27.650 | -6.387 | 1.000 | 26.00 |
| ATOM | 1988 | CA  | ASP A 269 | -6.096  | 28.750 | -7.019 | 1.000 | 24.51 |
| ATOM | 1989 | CB  | ASP A 269 | -6.616  | 28.978 | -8.444 | 1.000 | 36.81 |
| ATOM | 1990 | CG  | ASP A 269 | -8.072  | 29.337 | -8.608 | 1.000 | 32.33 |
| ATOM | 1991 | OD1 | ASP A 269 | -8.854  | 29.152 | -7.660 | 1.000 | 26.79 |
| ATOM | 1992 | OD2 | ASP A 269 | -8.465  | 29.822 | -9.701 | 1.000 | 28.81 |
| ATOM | 1993 | C   | ASP A 269 | -6.126  | 30.000 | -6.165 | 1.000 | 21.36 |
| ATOM | 1994 | O   | ASP A 269 | -5.857  | 31.124 | -6.623 | 1.000 | 25.20 |
| ATOM | 1995 | N   | SER A 270 | -6.434  | 29.846 | -4.867 | 1.000 | 19.08 |
| ATOM | 1996 | CA  | SER A 270 | -6.204  | 30.978 | -3.973 | 1.000 | 22.27 |
| ATOM | 1997 | CB  | SER A 270 | -7.455  | 31.809 | -3.722 | 1.000 | 31.53 |
| ATOM | 1998 | OG  | SER A 270 | -8.466  | 31.045 | -3.109 | 1.000 | 46.83 |
| ATOM | 1999 | C   | SER A 270 | -5.632  | 30.493 | -2.626 | 1.000 | 17.38 |
| ATOM | 2000 | O   | SER A 270 | -5.828  | 29.315 | -2.334 | 1.000 | 22.28 |
| ATOM | 2001 | N   | VAL A 271 | -5.000  | 31.394 | -1.910 | 1.000 | 20.10 |
| ATOM | 2002 | CA  | VAL A 271 | -4.413  | 31.067 | -0.596 | 1.000 | 21.99 |
| ATOM | 2003 | CB  | VAL A 271 | -2.876  | 31.020 | -0.706 | 1.000 | 36.16 |
| ATOM | 2004 | CG1 | VAL A 271 | -2.305  | 32.413 | -0.921 | 1.000 | 35.70 |
| ATOM | 2005 | CG2 | VAL A 271 | -2.233  | 30.370 | 0.514  | 1.000 | 31.05 |
| ATOM | 2006 | C   | VAL A 271 | -4.845  | 32.054 | 0.464  | 1.000 | 23.10 |
| ATOM | 2007 | O   | VAL A 271 | -5.012  | 33.251 | 0.241  | 1.000 | 21.67 |
| ATOM | 2008 | N   | ASP A 272 | -5.046  | 31.547 | 1.689  | 1.000 | 22.69 |
| ATOM | 2009 | CA  | ASP A 272 | -5.591  | 32.427 | 2.728  | 1.000 | 29.48 |
| ATOM | 2010 | CB  | ASP A 272 | -7.070  | 32.095 | 2.910  | 1.000 | 26.70 |
| ATOM | 2011 | CG  | ASP A 272 | -7.813  | 32.991 | 3.869  | 1.000 | 27.37 |
| ATOM | 2012 | OD1 | ASP A 272 | -7.274  | 34.038 | 4.288  | 1.000 | 23.01 |
| ATOM | 2013 | OD2 | ASP A 272 | -8.973  | 32.599 | 4.175  | 1.000 | 25.43 |
| ATOM | 2014 | C   | ASP A 272 | -4.807  | 32.259 | 4.021  | 1.000 | 22.94 |
| ATOM | 2015 | O   | ASP A 272 | -5.200  | 31.536 | 4.930  | 1.000 | 19.80 |
| ATOM | 2016 | N   | ILE A 273 | -3.661  | 32.934 | 4.069  | 1.000 | 24.25 |
| ATOM | 2017 | CA  | ILE A 273 | -2.806  | 32.829 | 5.255  | 1.000 | 22.39 |
| ATOM | 2018 | CB  | ILE A 273 | -1.436  | 33.465 | 4.962  | 1.000 | 25.49 |
| ATOM | 2019 | CG1 | ILE A 273 | -0.747  | 32.812 | 3.755  | 1.000 | 18.59 |
| ATOM | 2020 | CD1 | ILE A 273 | 0.498   | 33.584 | 3.329  | 1.000 | 24.40 |
| ATOM | 2021 | CG2 | ILE A 273 | -0.532  | 33.454 | 6.177  | 1.000 | 18.07 |
| ATOM | 2022 | C   | ILE A 273 | -3.472  | 33.457 | 6.452  | 1.000 | 20.71 |
| ATOM | 2023 | O   | ILE A 273 | -3.470  | 32.853 | 7.530  | 1.000 | 17.55 |
| ATOM | 2024 | N   | TYR A 274 | -4.038  | 34.646 | 6.266  | 1.000 | 21.57 |
| ATOM | 2025 | CA  | TYR A 274 | -4.765  | 35.332 | 7.338  | 1.000 | 27.63 |
| ATOM | 2026 | CB  | TYR A 274 | -5.414  | 36.646 | 6.864  | 1.000 | 23.61 |
| ATOM | 2027 | CG  | TYR A 274 | -6.110  | 37.456 | 7.937  | 1.000 | 24.88 |

**FIGURE 240**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |         |        |        |       |       |
|------|------|-----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 2028 | CD1 | TYR | A | 274 | -7.427  | 37.236 | 8.347  | 1.000 | 25.22 |
| ATOM | 2029 | CE1 | TYR | A | 274 | -8.040  | 37.979 | 9.328  | 1.000 | 24.84 |
| ATOM | 2030 | CZ  | TYR | A | 274 | -7.346  | 39.009 | 9.937  | 1.000 | 24.82 |
| ATOM | 2031 | OH  | TYR | A | 274 | -7.979  | 39.740 | 10.919 | 1.000 | 31.02 |
| ATOM | 2032 | CE2 | TYR | A | 274 | -6.040  | 39.266 | 9.571  | 1.000 | 24.34 |
| ATOM | 2033 | CD2 | TYR | A | 274 | -5.435  | 38.503 | 8.582  | 1.000 | 21.36 |
| ATOM | 2034 | C   | TYR | A | 274 | -5.834  | 34.413 | 7.922  | 1.000 | 22.02 |
| ATOM | 2035 | O   | TYR | A | 274 | -5.962  | 34.308 | 9.150  | 1.000 | 23.59 |
| ATOM | 2036 | N   | GLY | A | 275 | -6.642  | 33.818 | 7.042  | 1.000 | 19.06 |
| ATOM | 2037 | CA  | GLY | A | 275 | -7.741  | 32.997 | 7.563  | 1.000 | 18.44 |
| ATOM | 2038 | C   | GLY | A | 275 | -7.221  | 31.755 | 8.284  | 1.000 | 18.35 |
| ATOM | 2039 | O   | GLY | A | 275 | -7.789  | 31.310 | 9.278  | 1.000 | 20.87 |
| ATOM | 2040 | N   | ALA | A | 276 | -6.123  | 31.168 | 7.823  | 1.000 | 19.89 |
| ATOM | 2041 | CA  | ALA | A | 276 | -5.591  | 30.008 | 8.560  | 1.000 | 22.21 |
| ATOM | 2042 | CB  | ALA | A | 276 | -4.480  | 29.371 | 7.758  | 1.000 | 17.74 |
| ATOM | 2043 | C   | ALA | A | 276 | -5.091  | 30.429 | 9.932  | 1.000 | 24.08 |
| ATOM | 2044 | O   | ALA | A | 276 | -5.321  | 29.770 | 10.938 | 1.000 | 19.77 |
| ATOM | 2045 | N   | VAL | A | 277 | -4.390  | 31.569 | 10.019 | 1.000 | 18.02 |
| ATOM | 2046 | CA  | VAL | A | 277 | -3.912  | 31.978 | 11.353 | 1.000 | 17.46 |
| ATOM | 2047 | CB  | VAL | A | 277 | -2.831  | 33.079 | 11.246 | 1.000 | 21.08 |
| ATOM | 2048 | CG1 | VAL | A | 277 | -2.405  | 33.553 | 12.631 | 1.000 | 21.06 |
| ATOM | 2049 | CG2 | VAL | A | 277 | -1.645  | 32.548 | 10.467 | 1.000 | 16.97 |
| ATOM | 2050 | C   | VAL | A | 277 | -5.084  | 32.426 | 12.205 | 1.000 | 20.56 |
| ATOM | 2051 | O   | VAL | A | 277 | -5.142  | 32.112 | 13.390 | 1.000 | 18.55 |
| ATOM | 2052 | N   | HIS | A | 278 | -6.044  | 33.156 | 11.644 | 1.000 | 18.91 |
| ATOM | 2053 | CA  | HIS | A | 278 | -7.281  | 33.470 | 12.314 | 1.000 | 16.67 |
| ATOM | 2054 | CB  | HIS | A | 278 | -8.297  | 34.063 | 11.303 | 1.000 | 18.69 |
| ATOM | 2055 | CG  | HIS | A | 278 | -9.520  | 34.540 | 12.036 | 1.000 | 22.21 |
| ATOM | 2056 | ND1 | HIS | A | 278 | -10.626 | 33.756 | 12.252 | 1.000 | 21.90 |
| ATOM | 2057 | CE1 | HIS | A | 278 | -11.535 | 34.445 | 12.925 | 1.000 | 23.09 |
| ATOM | 2058 | NE2 | HIS | A | 278 | -11.055 | 35.656 | 13.150 | 1.000 | 23.99 |
| ATOM | 2059 | CD2 | HIS | A | 278 | -9.801  | 35.745 | 12.602 | 1.000 | 20.21 |
| ATOM | 2060 | C   | HIS | A | 278 | -7.924  | 32.254 | 12.971 | 1.000 | 19.90 |
| ATOM | 2061 | O   | HIS | A | 278 | -8.255  | 32.244 | 14.165 | 1.000 | 22.96 |
| ATOM | 2062 | N   | ASP | A | 279 | -8.105  | 31.202 | 12.180 | 1.000 | 18.82 |
| ATOM | 2063 | CA  | ASP | A | 279 | -8.742  | 30.004 | 12.711 | 1.000 | 23.67 |
| ATOM | 2064 | CB  | ASP | A | 279 | -8.995  | 29.015 | 11.565 | 1.000 | 25.00 |
| ATOM | 2065 | CG  | ASP | A | 279 | -10.100 | 29.571 | 10.669 | 1.000 | 50.27 |
| ATOM | 2066 | OD1 | ASP | A | 279 | -10.713 | 30.592 | 11.074 | 1.000 | 51.54 |
| ATOM | 2067 | OD2 | ASP | A | 279 | -10.315 | 28.989 | 9.582  | 1.000 | 44.55 |
| ATOM | 2068 | C   | ASP | A | 279 | -7.914  | 29.352 | 13.811 | 1.000 | 21.55 |
| ATOM | 2069 | O   | ASP | A | 279 | -8.488  | 28.905 | 14.806 | 1.000 | 24.05 |
| ATOM | 2070 | N   | LEU | A | 280 | -6.595  | 29.300 | 13.681 | 1.000 | 17.02 |
| ATOM | 2071 | CA  | LEU | A | 280 | -5.777  | 28.736 | 14.760 | 1.000 | 15.09 |
| ATOM | 2072 | CB  | LEU | A | 280 | -4.307  | 28.672 | 14.339 | 1.000 | 16.04 |
| ATOM | 2073 | CG  | LEU | A | 280 | -3.998  | 27.877 | 13.066 | 1.000 | 25.79 |
| ATOM | 2074 | CD1 | LEU | A | 280 | -2.505  | 27.860 | 12.743 | 1.000 | 19.03 |
| ATOM | 2075 | CD2 | LEU | A | 280 | -4.512  | 26.448 | 13.134 | 1.000 | 25.95 |
| ATOM | 2076 | C   | LEU | A | 280 | -5.928  | 29.541 | 16.041 | 1.000 | 17.95 |
| ATOM | 2077 | O   | LEU | A | 280 | -6.048  | 28.991 | 17.142 | 1.000 | 16.96 |
| ATOM | 2078 | N   | ARG | A | 281 | -5.940  | 30.867 | 15.909 | 1.000 | 17.70 |
| ATOM | 2079 | CA  | ARG | A | 281 | -6.048  | 31.750 | 17.064 | 1.000 | 20.80 |

**FIGURE 241**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |         |        |        |       |       |
|------|------|-----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 2080 | CB  | ARG | A | 281 | -5.937  | 33.220 | 16.611 | 1.000 | 16.23 |
| ATOM | 2081 | CG  | ARG | A | 281 | -4.518  | 33.577 | 16.185 | 1.000 | 21.03 |
| ATOM | 2082 | CD  | ARG | A | 281 | -3.551  | 33.775 | 17.350 | 1.000 | 20.13 |
| ATOM | 2083 | NE  | ARG | A | 281 | -2.333  | 34.410 | 16.826 | 1.000 | 22.94 |
| ATOM | 2084 | CZ  | ARG | A | 281 | -2.155  | 35.711 | 16.631 | 1.000 | 25.63 |
| ATOM | 2085 | NH1 | ARG | A | 281 | -3.096  | 36.606 | 16.909 | 1.000 | 26.26 |
| ATOM | 2086 | NH2 | ARG | A | 281 | -0.990  | 36.116 | 16.136 | 1.000 | 24.35 |
| ATOM | 2087 | C   | ARG | A | 281 | -7.348  | 31.512 | 17.810 | 1.000 | 18.17 |
| ATOM | 2088 | O   | ARG | A | 281 | -7.399  | 31.612 | 19.040 | 1.000 | 16.51 |
| ATOM | 2089 | N   | LEU | A | 282 | -8.411  | 31.197 | 17.055 | 1.000 | 14.33 |
| ATOM | 2090 | CA  | LEU | A | 282 | -9.670  | 30.904 | 17.725 | 1.000 | 19.27 |
| ATOM | 2091 | CB  | LEU | A | 282 | -10.750 | 30.565 | 16.690 | 1.000 | 19.77 |
| ATOM | 2092 | CG  | LEU | A | 282 | -11.369 | 31.764 | 15.966 | 1.000 | 29.93 |
| ATOM | 2093 | CD1 | LEU | A | 282 | -12.445 | 31.274 | 15.006 | 1.000 | 21.91 |
| ATOM | 2094 | CD2 | LEU | A | 282 | -11.916 | 32.785 | 16.951 | 1.000 | 25.11 |
| ATOM | 2095 | C   | LEU | A | 282 | -9.567  | 29.715 | 18.673 | 1.000 | 15.90 |
| ATOM | 2096 | O   | LEU | A | 282 | -10.343 | 29.644 | 19.622 | 1.000 | 19.86 |
| ATOM | 2097 | N   | HIS | A | 283 | -8.652  | 28.771 | 18.444 | 1.000 | 13.25 |
| ATOM | 2098 | CA  | HIS | A | 283 | -8.655  | 27.556 | 19.262 | 1.000 | 15.14 |
| ATOM | 2099 | CB  | HIS | A | 283 | -8.585  | 26.315 | 18.339 | 1.000 | 17.23 |
| ATOM | 2100 | CG  | HIS | A | 283 | -9.761  | 26.332 | 17.393 | 1.000 | 20.06 |
| ATOM | 2101 | ND1 | HIS | A | 283 | -10.931 | 25.651 | 17.625 | 1.000 | 31.88 |
| ATOM | 2102 | CE1 | HIS | A | 283 | -11.785 | 25.866 | 16.626 | 1.000 | 22.40 |
| ATOM | 2103 | NE2 | HIS | A | 283 | -11.210 | 26.665 | 15.743 | 1.000 | 22.21 |
| ATOM | 2104 | CD2 | HIS | A | 283 | -9.959  | 26.969 | 16.216 | 1.000 | 21.15 |
| ATOM | 2105 | C   | HIS | A | 283 | -7.541  | 27.484 | 20.301 | 1.000 | 17.70 |
| ATOM | 2106 | O   | HIS | A | 283 | -7.668  | 26.724 | 21.286 | 1.000 | 18.21 |
| ATOM | 2107 | N   | ARG | A | 284 | -6.460  | 28.254 | 20.155 | 1.000 | 18.34 |
| ATOM | 2108 | CA  | ARG | A | 284 | -5.462  | 28.288 | 21.252 | 1.000 | 17.74 |
| ATOM | 2109 | CB  | ARG | A | 284 | -4.494  | 27.114 | 21.172 | 1.000 | 19.63 |
| ATOM | 2110 | CG  | ARG | A | 284 | -3.445  | 26.954 | 22.275 | 1.000 | 18.29 |
| ATOM | 2111 | CD  | ARG | A | 284 | -2.651  | 25.656 | 22.082 | 1.000 | 20.72 |
| ATOM | 2112 | NE  | ARG | A | 284 | -1.458  | 25.545 | 22.957 | 1.000 | 15.01 |
| ATOM | 2113 | CZ  | ARG | A | 284 | -1.489  | 25.046 | 24.189 | 1.000 | 14.81 |
| ATOM | 2114 | NH1 | ARG | A | 284 | -2.637  | 24.611 | 24.697 | 1.000 | 14.36 |
| ATOM | 2115 | NH2 | ARG | A | 284 | -0.419  | 24.947 | 24.977 | 1.000 | 17.97 |
| ATOM | 2116 | C   | ARG | A | 284 | -4.746  | 29.631 | 21.220 | 1.000 | 19.40 |
| ATOM | 2117 | O   | ARG | A | 284 | -4.570  | 30.222 | 20.158 | 1.000 | 18.68 |
| ATOM | 2118 | N   | VAL | A | 285 | -4.331  | 30.137 | 22.382 | 1.000 | 20.56 |
| ATOM | 2119 | CA  | VAL | A | 285 | -3.577  | 31.396 | 22.467 | 1.000 | 19.97 |
| ATOM | 2120 | CB  | VAL | A | 285 | -3.329  | 31.773 | 23.942 | 1.000 | 20.57 |
| ATOM | 2121 | CG1 | VAL | A | 285 | -2.329  | 30.829 | 24.584 | 1.000 | 17.50 |
| ATOM | 2122 | CG2 | VAL | A | 285 | -2.811  | 33.203 | 24.085 | 1.000 | 29.47 |
| ATOM | 2123 | C   | VAL | A | 285 | -2.259  | 31.298 | 21.714 | 1.000 | 17.66 |
| ATOM | 2124 | O   | VAL | A | 285 | -1.641  | 30.232 | 21.618 | 1.000 | 17.67 |
| ATOM | 2125 | N   | HIS | A | 286 | -1.814  | 32.423 | 21.166 | 1.000 | 19.91 |
| ATOM | 2126 | CA  | HIS | A | 286 | -0.537  | 32.572 | 20.510 | 1.000 | 25.50 |
| ATOM | 2127 | CB  | HIS | A | 286 | 0.610   | 32.334 | 21.518 | 1.000 | 24.01 |
| ATOM | 2128 | CG  | HIS | A | 286 | 0.534   | 33.321 | 22.640 | 1.000 | 27.47 |
| ATOM | 2129 | ND1 | HIS | A | 286 | 0.673   | 32.943 | 23.966 | 1.000 | 36.12 |
| ATOM | 2130 | CE1 | HIS | A | 286 | 0.544   | 34.024 | 24.711 | 1.000 | 31.77 |
| ATOM | 2131 | NE2 | HIS | A | 286 | 0.333   | 35.065 | 23.927 | 1.000 | 32.36 |

**FIGURE 242**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2132 | CD2 | HIS | A | 286 | 0.312  | 34.647 | 22.624 | 1.000 | 25.03 |
| ATOM | 2133 | C   | HIS | A | 286 | -0.272 | 31.626 | 19.358 | 1.000 | 21.57 |
| ATOM | 2134 | O   | HIS | A | 286 | 0.915  | 31.389 | 19.095 | 1.000 | 27.54 |
| ATOM | 2135 | N   | MET | A | 287 | -1.298 | 31.074 | 18.700 | 1.000 | 20.51 |
| ATOM | 2136 | CA  | MET | A | 287 | -1.005 | 30.215 | 17.540 | 1.000 | 17.32 |
| ATOM | 2137 | CB  | MET | A | 287 | -2.248 | 29.446 | 17.099 | 1.000 | 15.20 |
| ATOM | 2138 | CG  | MET | A | 287 | -2.726 | 28.475 | 18.174 | 1.000 | 18.71 |
| ATOM | 2139 | SD  | MET | A | 287 | -1.588 | 27.070 | 18.339 | 1.000 | 23.88 |
| ATOM | 2140 | CE  | MET | A | 287 | -2.087 | 26.118 | 16.902 | 1.000 | 40.45 |
| ATOM | 2141 | C   | MET | A | 287 | -0.449 | 31.093 | 16.419 | 1.000 | 19.40 |
| ATOM | 2142 | O   | MET | A | 287 | -1.200 | 31.865 | 15.805 | 1.000 | 23.59 |
| ATOM | 2143 | N   | VAL | A | 288 | 0.842  | 30.986 | 16.169 | 1.000 | 18.22 |
| ATOM | 2144 | CA  | VAL | A | 288 | 1.568  | 31.941 | 15.322 | 1.000 | 22.64 |
| ATOM | 2145 | CB  | VAL | A | 288 | 0.926  | 32.326 | 13.986 | 1.000 | 17.14 |
| ATOM | 2146 | CG1 | VAL | A | 288 | 1.879  | 33.209 | 13.183 | 1.000 | 23.13 |
| ATOM | 2147 | CG2 | VAL | A | 288 | 0.607  | 31.099 | 13.159 | 1.000 | 21.03 |
| ATOM | 2148 | C   | VAL | A | 288 | 1.718  | 33.186 | 16.211 | 1.000 | 25.94 |
| ATOM | 2149 | O   | VAL | A | 288 | 0.851  | 34.046 | 16.243 | 1.000 | 27.22 |
| ATOM | 2150 | N   | GLN | A | 289 | 2.824  | 33.161 | 16.945 | 1.000 | 27.43 |
| ATOM | 2151 | CA  | GLN | A | 289 | 3.003  | 34.056 | 18.091 | 1.000 | 24.77 |
| ATOM | 2152 | CB  | GLN | A | 289 | 3.839  | 33.286 | 19.112 | 1.000 | 23.16 |
| ATOM | 2153 | CG  | GLN | A | 289 | 4.041  | 33.984 | 20.443 | 1.000 | 22.98 |
| ATOM | 2154 | CD  | GLN | A | 289 | 4.639  | 33.050 | 21.469 | 1.000 | 24.02 |
| ATOM | 2155 | OE1 | GLN | A | 289 | 5.224  | 32.012 | 21.115 | 1.000 | 27.34 |
| ATOM | 2156 | NE2 | GLN | A | 289 | 4.479  | 33.454 | 22.716 | 1.000 | 30.58 |
| ATOM | 2157 | C   | GLN | A | 289 | 3.664  | 35.376 | 17.751 | 1.000 | 28.02 |
| ATOM | 2158 | O   | GLN | A | 289 | 3.430  | 36.375 | 18.436 | 1.000 | 35.00 |
| ATOM | 2159 | N   | THR | A | 290 | 4.492  | 35.409 | 16.717 | 1.000 | 22.20 |
| ATOM | 2160 | CA  | THR | A | 290 | 5.169  | 36.667 | 16.419 | 1.000 | 24.68 |
| ATOM | 2161 | CB  | THR | A | 290 | 6.682  | 36.492 | 16.619 | 1.000 | 25.80 |
| ATOM | 2162 | OG1 | THR | A | 290 | 7.133  | 35.616 | 15.579 | 1.000 | 22.41 |
| ATOM | 2163 | CG2 | THR | A | 290 | 7.012  | 35.803 | 17.932 | 1.000 | 28.39 |
| ATOM | 2164 | C   | THR | A | 290 | 4.964  | 37.120 | 14.984 | 1.000 | 35.97 |
| ATOM | 2165 | O   | THR | A | 290 | 4.668  | 36.327 | 14.090 | 1.000 | 25.80 |
| ATOM | 2166 | N   | GLU | A | 291 | 5.148  | 38.416 | 14.746 | 1.000 | 29.48 |
| ATOM | 2167 | CA  | GLU | A | 291 | 5.038  | 38.965 | 13.403 | 1.000 | 28.57 |
| ATOM | 2168 | CB  | GLU | A | 291 | 5.285  | 40.473 | 13.478 | 1.000 | 29.75 |
| ATOM | 2169 | CG  | GLU | A | 291 | 5.073  | 41.210 | 12.184 | 1.000 | 39.81 |
| ATOM | 2170 | CD  | GLU | A | 291 | 4.812  | 42.699 | 12.387 | 1.000 | 39.37 |
| ATOM | 2171 | OE1 | GLU | A | 291 | 4.858  | 43.418 | 11.371 | 1.000 | 42.29 |
| ATOM | 2172 | OE2 | GLU | A | 291 | 4.556  | 43.148 | 13.519 | 1.000 | 40.22 |
| ATOM | 2173 | C   | GLU | A | 291 | 6.029  | 38.283 | 12.484 | 1.000 | 23.04 |
| ATOM | 2174 | O   | GLU | A | 291 | 5.824  | 37.994 | 11.304 | 1.000 | 23.87 |
| ATOM | 2175 | N   | CYS | A | 292 | 7.200  | 37.987 | 13.054 | 1.000 | 24.91 |
| ATOM | 2176 | CA  | CYS | A | 292 | 8.230  | 37.313 | 12.255 | 1.000 | 20.83 |
| ATOM | 2177 | CB  | CYS | A | 292 | 9.434  | 37.106 | 13.178 | 1.000 | 33.84 |
| ATOM | 2178 | SG  | CYS | A | 292 | 10.875 | 36.380 | 12.364 | 1.000 | 50.67 |
| ATOM | 2179 | C   | CYS | A | 292 | 7.777  | 35.977 | 11.679 | 1.000 | 25.36 |
| ATOM | 2180 | O   | CYS | A | 292 | 8.056  | 35.544 | 10.549 | 1.000 | 26.36 |
| ATOM | 2181 | N   | GLN | A | 293 | 7.024  | 35.250 | 12.515 | 1.000 | 23.19 |
| ATOM | 2182 | CA  | GLN | A | 293 | 6.425  | 33.998 | 12.069 | 1.000 | 22.92 |
| ATOM | 2183 | CB  | GLN | A | 293 | 5.779  | 33.269 | 13.256 | 1.000 | 20.65 |

**FIGURE 243**

|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2184 | CG  | GLN | A | 293 | 6.783  | 32.437 | 14.036 | 1.000 | 20.24 |
| ATOM | 2185 | CD  | GLN | A | 293 | 6.355  | 32.071 | 15.433 | 1.000 | 17.59 |
| ATOM | 2186 | OE1 | GLN | A | 293 | 5.282  | 32.450 | 15.901 | 1.000 | 18.69 |
| ATOM | 2187 | NE2 | GLN | A | 293 | 7.203  | 31.336 | 16.150 | 1.000 | 25.13 |
| ATOM | 2188 | C   | GLN | A | 293 | 5.400  | 34.266 | 10.967 | 1.000 | 17.64 |
| ATOM | 2189 | O   | GLN | A | 293 | 5.398  | 33.582 | 9.954  | 1.000 | 20.18 |
| ATOM | 2190 | N   | TYR | A | 294 | 4.522  | 35.253 | 11.178 | 1.000 | 20.42 |
| ATOM | 2191 | CA  | TYR | A | 294 | 3.526  | 35.600 | 10.153 | 1.000 | 19.65 |
| ATOM | 2192 | CB  | TYR | A | 294 | 2.680  | 36.758 | 10.698 | 1.000 | 19.00 |
| ATOM | 2193 | CG  | TYR | A | 294 | 1.392  | 36.980 | 9.943  | 1.000 | 21.07 |
| ATOM | 2194 | CD1 | TYR | A | 294 | 0.438  | 35.986 | 9.843  | 1.000 | 19.94 |
| ATOM | 2195 | CE1 | TYR | A | 294 | -0.747 | 36.155 | 9.158  | 1.000 | 25.08 |
| ATOM | 2196 | CZ  | TYR | A | 294 | -0.978 | 37.374 | 8.547  | 1.000 | 34.68 |
| ATOM | 2197 | OH  | TYR | A | 294 | -2.148 | 37.565 | 7.856  | 1.000 | 23.20 |
| ATOM | 2198 | CE2 | TYR | A | 294 | -0.047 | 38.385 | 8.622  | 1.000 | 26.61 |
| ATOM | 2199 | CD2 | TYR | A | 294 | 1.129  | 38.197 | 9.316  | 1.000 | 23.82 |
| ATOM | 2200 | C   | TYR | A | 294 | 4.202  | 35.931 | 8.834  | 1.000 | 24.14 |
| ATOM | 2201 | O   | TYR | A | 294 | 3.860  | 35.493 | 7.737  | 1.000 | 23.97 |
| ATOM | 2202 | N   | VAL | A | 295 | 5.254  | 36.744 | 8.919  | 1.000 | 25.60 |
| ATOM | 2203 | CA  | VAL | A | 295 | 6.065  | 37.085 | 7.762  | 1.000 | 26.06 |
| ATOM | 2204 | CB  | VAL | A | 295 | 7.222  | 38.039 | 8.161  | 1.000 | 22.22 |
| ATOM | 2205 | CG1 | VAL | A | 295 | 8.189  | 38.107 | 6.995  | 1.000 | 24.48 |
| ATOM | 2206 | CG2 | VAL | A | 295 | 6.668  | 39.400 | 8.553  | 1.000 | 22.52 |
| ATOM | 2207 | C   | VAL | A | 295 | 6.648  | 35.853 | 7.111  | 1.000 | 20.01 |
| ATOM | 2208 | O   | VAL | A | 295 | 6.582  | 35.637 | 5.897  | 1.000 | 23.07 |
| ATOM | 2209 | N   | TYR | A | 296 | 7.233  | 34.941 | 7.888  | 1.000 | 29.06 |
| ATOM | 2210 | CA  | TYR | A | 296 | 7.779  | 33.698 | 7.342  | 1.000 | 20.10 |
| ATOM | 2211 | CB  | TYR | A | 296 | 8.307  | 32.873 | 8.528  | 1.000 | 20.14 |
| ATOM | 2212 | CG  | TYR | A | 296 | 9.099  | 31.652 | 8.140  | 1.000 | 22.62 |
| ATOM | 2213 | CD1 | TYR | A | 296 | 10.343 | 31.723 | 7.536  | 1.000 | 24.11 |
| ATOM | 2214 | CE1 | TYR | A | 296 | 11.044 | 30.582 | 7.188  | 1.000 | 24.78 |
| ATOM | 2215 | CZ  | TYR | A | 296 | 10.500 | 29.338 | 7.451  | 1.000 | 30.65 |
| ATOM | 2216 | OH  | TYR | A | 296 | 11.171 | 28.185 | 7.115  | 1.000 | 25.95 |
| ATOM | 2217 | CE2 | TYR | A | 296 | 9.263  | 29.241 | 8.048  | 1.000 | 21.75 |
| ATOM | 2218 | CD2 | TYR | A | 296 | 8.570  | 30.384 | 8.389  | 1.000 | 22.93 |
| ATOM | 2219 | C   | TYR | A | 296 | 6.802  | 32.832 | 6.546  | 1.000 | 19.59 |
| ATOM | 2220 | O   | TYR | A | 296 | 7.163  | 32.193 | 5.540  | 1.000 | 20.16 |
| ATOM | 2221 | N   | LEU | A | 297 | 5.555  | 32.742 | 6.984  | 1.000 | 21.48 |
| ATOM | 2222 | CA  | LEU | A | 297 | 4.501  | 32.003 | 6.276  | 1.000 | 16.66 |
| ATOM | 2223 | CB  | LEU | A | 297 | 3.186  | 31.985 | 7.052  | 1.000 | 17.75 |
| ATOM | 2224 | CG  | LEU | A | 297 | 3.215  | 31.148 | 8.360  | 1.000 | 16.83 |
| ATOM | 2225 | CD1 | LEU | A | 297 | 2.035  | 31.495 | 9.235  | 1.000 | 17.79 |
| ATOM | 2226 | CD2 | LEU | A | 297 | 3.299  | 29.668 | 8.014  | 1.000 | 17.48 |
| ATOM | 2227 | C   | LEU | A | 297 | 4.276  | 32.654 | 4.904  | 1.000 | 17.96 |
| ATOM | 2228 | O   | LEU | A | 297 | 4.156  | 31.967 | 3.898  | 1.000 | 20.64 |
| ATOM | 2229 | N   | HIS | A | 298 | 4.256  | 33.978 | 4.931  | 1.000 | 22.58 |
| ATOM | 2230 | CA  | HIS | A | 298 | 4.152  | 34.678 | 3.633  | 1.000 | 23.47 |
| ATOM | 2231 | CB  | HIS | A | 298 | 3.950  | 36.157 | 3.901  | 1.000 | 25.50 |
| ATOM | 2232 | CG  | HIS | A | 298 | 2.562  | 36.496 | 4.341  | 1.000 | 26.24 |
| ATOM | 2233 | ND1 | HIS | A | 298 | 2.118  | 36.313 | 5.625  | 1.000 | 22.98 |
| ATOM | 2234 | CE1 | HIS | A | 298 | 0.865  | 36.709 | 5.744  | 1.000 | 24.82 |
| ATOM | 2235 | NE2 | HIS | A | 298 | 0.470  | 37.141 | 4.565  | 1.000 | 27.56 |

**FIGURE 244**



|      |      |     |     |   |     |        |        |        |       |       |
|------|------|-----|-----|---|-----|--------|--------|--------|-------|-------|
| ATOM | 2236 | CD2 | HIS | A | 298 | 1.512  | 37.022 | 3.673  | 1.000 | 23.83 |
| ATOM | 2237 | C   | HIS | A | 298 | 5.379  | 34.412 | 2.785  | 1.000 | 20.56 |
| ATOM | 2238 | O   | HIS | A | 298 | 5.260  | 34.132 | 1.597  | 1.000 | 21.25 |
| ATOM | 2239 | N   | GLN | A | 299 | 6.602  | 34.457 | 3.323  | 1.000 | 24.45 |
| ATOM | 2240 | CA  | GLN | A | 299 | 7.767  | 34.186 | 2.484  | 1.000 | 23.57 |
| ATOM | 2241 | CB  | GLN | A | 299 | 9.094  | 34.286 | 3.248  | 1.000 | 24.20 |
| ATOM | 2242 | CG  | GLN | A | 299 | 9.618  | 35.701 | 3.344  | 1.000 | 38.95 |
| ATOM | 2243 | CD  | GLN | A | 299 | 10.513 | 35.927 | 4.544  | 1.000 | 41.27 |
| ATOM | 2244 | OE1 | GLN | A | 299 | 10.525 | 35.111 | 5.469  | 1.000 | 47.05 |
| ATOM | 2245 | NE2 | GLN | A | 299 | 11.230 | 37.044 | 4.501  | 1.000 | 36.99 |
| ATOM | 2246 | C   | GLN | A | 299 | 7.706  | 32.790 | 1.911  | 1.000 | 17.62 |
| ATOM | 2247 | O   | GLN | A | 299 | 8.136  | 32.450 | 0.809  | 1.000 | 25.21 |
| ATOM | 2248 | N   | CYS | A | 300 | 7.152  | 31.871 | 2.733  | 1.000 | 23.78 |
| ATOM | 2249 | CA  | CYS | A | 300 | 7.113  | 30.506 | 2.245  | 1.000 | 15.17 |
| ATOM | 2250 | CB  | CYS | A | 300 | 6.555  | 29.579 | 3.330  | 1.000 | 26.74 |
| ATOM | 2251 | SG  | CYS | A | 300 | 7.710  | 29.138 | 4.647  | 1.000 | 25.71 |
| ATOM | 2252 | C   | CYS | A | 300 | 6.212  | 30.350 | 1.023  | 1.000 | 21.29 |
| ATOM | 2253 | O   | CYS | A | 300 | 6.539  | 29.695 | 0.050  | 1.000 | 24.33 |
| ATOM | 2254 | N   | VAL | A | 301 | 5.033  | 30.956 | 1.118  | 1.000 | 22.72 |
| ATOM | 2255 | CA  | VAL | A | 301 | 4.112  | 30.918 | -0.014 | 1.000 | 22.06 |
| ATOM | 2256 | CB  | VAL | A | 301 | 2.771  | 31.522 | 0.407  | 1.000 | 23.59 |
| ATOM | 2257 | CG1 | VAL | A | 301 | 1.869  | 31.780 | -0.793 | 1.000 | 27.41 |
| ATOM | 2258 | CG2 | VAL | A | 301 | 2.103  | 30.549 | 1.385  | 1.000 | 22.39 |
| ATOM | 2259 | C   | VAL | A | 301 | 4.739  | 31.650 | -1.213 | 1.000 | 26.22 |
| ATOM | 2260 | O   | VAL | A | 301 | 4.684  | 31.075 | -2.300 | 1.000 | 25.21 |
| ATOM | 2261 | N   | ARG | A | 302 | 5.299  | 32.832 | -0.941 | 1.000 | 30.33 |
| ATOM | 2262 | CA  | ARG | A | 302 | 5.937  | 33.614 | -2.013 | 1.000 | 27.54 |
| ATOM | 2263 | CB  | ARG | A | 302 | 6.701  | 34.808 | -1.462 | 1.000 | 26.63 |
| ATOM | 2264 | CG  | ARG | A | 302 | 7.324  | 35.658 | -2.568 | 1.000 | 39.21 |
| ATOM | 2265 | CD  | ARG | A | 302 | 8.529  | 36.449 | -2.082 | 1.000 | 43.43 |
| ATOM | 2266 | NE  | ARG | A | 302 | 9.554  | 35.568 | -1.510 | 1.000 | 37.14 |
| ATOM | 2267 | CZ  | ARG | A | 302 | 10.329 | 35.931 | -0.494 | 1.000 | 41.54 |
| ATOM | 2268 | NH1 | ARG | A | 302 | 10.197 | 37.132 | 0.049  | 1.000 | 63.42 |
| ATOM | 2269 | NH2 | ARG | A | 302 | 11.233 | 35.083 | -0.027 | 1.000 | 50.68 |
| ATOM | 2270 | C   | ARG | A | 302 | 6.895  | 32.701 | -2.764 | 1.000 | 32.29 |
| ATOM | 2271 | O   | ARG | A | 302 | 6.982  | 32.557 | -3.972 | 1.000 | 31.68 |
| ATOM | 2272 | N   | ASP | A | 303 | 7.670  | 31.982 | -1.931 | 1.000 | 27.62 |
| ATOM | 2273 | CA  | ASP | A | 303 | 8.736  | 31.200 | -2.547 | 1.000 | 23.05 |
| ATOM | 2274 | CB  | ASP | A | 303 | 9.749  | 30.722 | -1.496 | 1.000 | 29.94 |
| ATOM | 2275 | CG  | ASP | A | 303 | 10.561 | 31.886 | -0.934 | 1.000 | 44.96 |
| ATOM | 2276 | OD1 | ASP | A | 303 | 10.575 | 33.000 | -1.513 | 1.000 | 37.48 |
| ATOM | 2277 | OD2 | ASP | A | 303 | 11.207 | 31.698 | 0.125  | 1.000 | 27.41 |
| ATOM | 2278 | C   | ASP | A | 303 | 8.159  | 30.064 | -3.366 | 1.000 | 32.89 |
| ATOM | 2279 | O   | ASP | A | 303 | 8.647  | 29.887 | -4.490 | 1.000 | 34.89 |
| ATOM | 2280 | N   | VAL | A | 304 | 7.167  | 29.345 | -2.844 | 1.000 | 30.50 |
| ATOM | 2281 | CA  | VAL | A | 304 | 6.548  | 28.260 | -3.598 | 1.000 | 23.94 |
| ATOM | 2282 | CB  | VAL | A | 304 | 5.491  | 27.493 | -2.783 | 1.000 | 27.62 |
| ATOM | 2283 | CG1 | VAL | A | 304 | 4.652  | 26.589 | -3.669 | 1.000 | 23.38 |
| ATOM | 2284 | CG2 | VAL | A | 304 | 6.165  | 26.665 | -1.692 | 1.000 | 24.59 |
| ATOM | 2285 | C   | VAL | A | 304 | 5.884  | 28.774 | -4.877 | 1.000 | 22.14 |
| ATOM | 2286 | O   | VAL | A | 304 | 6.042  | 28.169 | -5.933 | 1.000 | 25.47 |
| ATOM | 2287 | N   | LEU | A | 305 | 5.140  | 29.874 | -4.827 | 1.000 | 27.71 |

**FIGURE 245**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |         |       |       |
|------|------|-----|-----|---|-----|--------|--------|---------|-------|-------|
| ATOM | 2288 | CA  | LEU | A | 305 | 4.558  | 30.400 | -6.073  | 1.000 | 29.38 |
| ATOM | 2289 | CB  | LEU | A | 305 | 3.555  | 31.506 | -5.706  | 1.000 | 38.16 |
| ATOM | 2290 | CG  | LEU | A | 305 | 2.392  | 31.001 | -4.830  | 1.000 | 35.13 |
| ATOM | 2291 | CD1 | LEU | A | 305 | 1.344  | 32.082 | -4.643  | 1.000 | 31.50 |
| ATOM | 2292 | CD2 | LEU | A | 305 | 1.810  | 29.740 | -5.458  | 1.000 | 27.65 |
| ATOM | 2293 | C   | LEU | A | 305 | 5.606  | 30.942 | -7.043  | 1.000 | 39.73 |
| ATOM | 2294 | O   | LEU | A | 305 | 5.477  | 30.795 | -8.267  | 1.000 | 34.97 |
| ATOM | 2295 | N   | ARG | A | 306 | 6.644  | 31.587 | -6.500  | 1.000 | 30.15 |
| ATOM | 2296 | CA  | ARG | A | 306 | 7.696  | 32.191 | -7.303  | 1.000 | 41.94 |
| ATOM | 2297 | CB  | ARG | A | 306 | 8.843  | 32.715 | -6.443  | 1.000 | 44.09 |
| ATOM | 2298 | CG  | ARG | A | 306 | 9.589  | 33.889 | -7.052  | 1.000 | 39.22 |
| ATOM | 2299 | CD  | ARG | A | 306 | 10.448 | 34.547 | -5.980  | 1.000 | 42.72 |
| ATOM | 2300 | NE  | ARG | A | 306 | 9.979  | 35.884 | -5.635  | 1.000 | 52.78 |
| ATOM | 2301 | CZ  | ARG | A | 306 | 10.606 | 36.671 | -4.767  | 1.000 | 54.00 |
| ATOM | 2302 | NH1 | ARG | A | 306 | 11.714 | 36.247 | -4.169  | 1.000 | 67.12 |
| ATOM | 2303 | NH2 | ARG | A | 306 | 10.130 | 37.875 | -4.496  | 1.000 | 46.01 |
| ATOM | 2304 | C   | ARG | A | 306 | 8.287  | 31.172 | -8.271  | 1.000 | 29.94 |
| ATOM | 2305 | O   | ARG | A | 306 | 8.462  | 31.437 | -9.450  | 1.000 | 37.35 |
| ATOM | 2306 | N   | ALA | A | 307 | 8.569  | 30.025 | -7.699  | 1.000 | 31.66 |
| ATOM | 2307 | CA  | ALA | A | 307 | 9.158  | 28.861 | -8.317  | 1.000 | 23.60 |
| ATOM | 2308 | CB  | ALA | A | 307 | 9.447  | 27.819 | -7.233  | 1.000 | 26.10 |
| ATOM | 2309 | C   | ALA | A | 307 | 8.306  | 28.189 | -9.381  | 1.000 | 47.11 |
| ATOM | 2310 | O   | ALA | A | 307 | 8.799  | 28.044 | -10.499 | 1.000 | 44.35 |
| ATOM | 2311 | N   | ARG | A | 308 | 7.102  | 27.762 | -9.042  | 1.000 | 52.74 |
| ATOM | 2312 | CA  | ARG | A | 308 | 6.308  | 26.829 | -9.829  | 1.000 | 54.48 |
| ATOM | 2313 | CB  | ARG | A | 308 | 4.971  | 26.558 | -9.115  | 1.000 | 57.15 |
| ATOM | 2314 | CG  | ARG | A | 308 | 5.194  | 25.951 | -7.736  | 1.000 | 58.94 |
| ATOM | 2315 | CD  | ARG | A | 308 | 4.116  | 24.969 | -7.323  | 1.000 | 55.91 |
| ATOM | 2316 | NE  | ARG | A | 308 | 2.804  | 25.598 | -7.229  | 1.000 | 48.91 |
| ATOM | 2317 | CZ  | ARG | A | 308 | 1.773  | 25.117 | -6.536  | 1.000 | 51.64 |
| ATOM | 2318 | NH1 | ARG | A | 308 | 1.868  | 23.990 | -5.844  | 1.000 | 35.99 |
| ATOM | 2319 | NH2 | ARG | A | 308 | 0.639  | 25.806 | -6.558  | 1.000 | 44.89 |
| ATOM | 2320 | C   | ARG | A | 308 | 6.063  | 27.269 | -11.267 | 1.000 | 53.61 |
| ATOM | 2321 | O   | ARG | A | 308 | 5.807  | 26.391 | -12.115 | 1.000 | 48.27 |
| ATOM | 2322 | N   | LYS | A | 309 | 6.155  | 28.565 | -11.523 | 1.000 | 43.56 |
| ATOM | 2323 | CA  | LYS | A | 309 | 6.129  | 29.126 | -12.866 | 1.000 | 55.87 |
| ATOM | 2324 | CB  | LYS | A | 309 | 6.515  | 30.617 | -12.836 | 1.000 | 53.73 |
| ATOM | 2325 | CG  | LYS | A | 309 | 5.322  | 31.519 | -12.555 | 1.000 | 50.14 |
| ATOM | 2326 | CD  | LYS | A | 309 | 5.733  | 32.861 | -11.988 | 1.000 | 51.79 |
| ATOM | 2327 | CE  | LYS | A | 309 | 5.194  | 33.994 | -12.859 | 1.000 | 58.07 |
| ATOM | 2328 | NZ  | LYS | A | 309 | 5.302  | 35.321 | -12.188 | 1.000 | 68.64 |
| ATOM | 2329 | C   | LYS | A | 309 | 7.071  | 28.394 | -13.819 | 1.000 | 49.69 |
| ATOM | 2330 | O   | LYS | A | 309 | 6.769  | 28.146 | -14.991 | 1.000 | 49.16 |
| ATOM | 2331 | N   | LEU | A | 310 | 8.259  | 28.052 | -13.326 | 1.000 | 28.26 |
| ATOM | 2332 | CA  | LEU | A | 310 | 9.179  | 27.229 | -14.104 | 1.000 | 38.83 |
| ATOM | 2333 | CB  | LEU | A | 310 | 10.617 | 27.612 | -13.747 | 1.000 | 55.29 |
| ATOM | 2334 | CG  | LEU | A | 310 | 10.793 | 29.062 | -13.278 | 1.000 | 62.65 |
| ATOM | 2335 | CD1 | LEU | A | 310 | 12.262 | 29.360 | -12.996 | 1.000 | 82.48 |
| ATOM | 2336 | CD2 | LEU | A | 310 | 10.245 | 30.039 | -14.295 | 1.000 | 58.72 |
| ATOM | 2337 | C   | LEU | A | 310 | 8.920  | 25.745 | -13.861 | 1.000 | 34.79 |
| ATOM | 2338 | O1  | HOH | W | 1   | 2.014  | 17.687 | 26.597  | 1.000 | 14.70 |
| ATOM | 2339 | O1  | HOH | W | 2   | -5.416 | 28.864 | 24.748  | 1.000 | 14.82 |

**FIGURE 246**

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Three Dimensional Coordinates of HPTPbeta

|      |      |    |     |   |    |         |        |        |       |       |
|------|------|----|-----|---|----|---------|--------|--------|-------|-------|
| ATOM | 2340 | O1 | HOH | W | 3  | 9.941   | 34.403 | 15.794 | 1.000 | 20.77 |
| ATOM | 2341 | O1 | HOH | W | 4  | 1.150   | 20.544 | 3.861  | 1.000 | 16.32 |
| ATOM | 2342 | O1 | HOH | W | 5  | 11.855  | 1.496  | 23.723 | 1.000 | 20.79 |
| ATOM | 2343 | O1 | HOH | W | 6  | 11.026  | 19.440 | 31.061 | 1.000 | 22.81 |
| ATOM | 2344 | O1 | HOH | W | 7  | -4.100  | 15.347 | 34.619 | 1.000 | 20.35 |
| ATOM | 2345 | O1 | HOH | W | 8  | -8.502  | 35.220 | 27.278 | 1.000 | 20.31 |
| ATOM | 2346 | O1 | HOH | W | 9  | 10.956  | 8.876  | 28.629 | 1.000 | 24.20 |
| ATOM | 2347 | O1 | HOH | W | 10 | 13.818  | 22.433 | 16.330 | 1.000 | 21.57 |
| ATOM | 2348 | O1 | HOH | W | 11 | -4.748  | 20.337 | 7.520  | 1.000 | 18.34 |
| ATOM | 2349 | O1 | HOH | W | 12 | 7.144   | 17.757 | 36.248 | 1.000 | 23.39 |
| ATOM | 2350 | O1 | HOH | W | 13 | -8.500  | 25.553 | 30.582 | 1.000 | 21.46 |
| ATOM | 2351 | O1 | HOH | W | 14 | 1.872   | 18.169 | 29.324 | 1.000 | 19.74 |
| ATOM | 2352 | O1 | HOH | W | 15 | -12.583 | 28.920 | 26.833 | 1.000 | 23.46 |
| ATOM | 2353 | O1 | HOH | W | 16 | 17.845  | 15.230 | 13.268 | 1.000 | 25.48 |
| ATOM | 2354 | O1 | HOH | W | 17 | 2.522   | 25.792 | 29.444 | 1.000 | 21.14 |
| ATOM | 2355 | O1 | HOH | W | 18 | -12.414 | 36.213 | 18.671 | 1.000 | 35.42 |
| ATOM | 2356 | O1 | HOH | W | 19 | -0.308  | 19.015 | 30.907 | 1.000 | 20.05 |
| ATOM | 2357 | O1 | HOH | W | 20 | -4.507  | 15.507 | 8.656  | 1.000 | 26.56 |
| ATOM | 2358 | O1 | HOH | W | 21 | -1.463  | 16.804 | 32.355 | 1.000 | 19.87 |
| ATOM | 2359 | O1 | HOH | W | 22 | -7.774  | 24.896 | 24.411 | 1.000 | 25.30 |
| ATOM | 2360 | O1 | HOH | W | 23 | 2.487   | 23.390 | -2.046 | 1.000 | 21.28 |
| ATOM | 2361 | O1 | HOH | W | 24 | -5.084  | 36.399 | 19.340 | 1.000 | 24.16 |
| ATOM | 2362 | O1 | HOH | W | 25 | 11.554  | 11.480 | 16.357 | 1.000 | 25.31 |
| ATOM | 2363 | O1 | HOH | W | 26 | 12.946  | 5.581  | 11.917 | 1.000 | 24.23 |
| ATOM | 2364 | O1 | HOH | W | 27 | -12.980 | 20.577 | 24.368 | 1.000 | 27.97 |
| ATOM | 2365 | O1 | HOH | W | 28 | 10.212  | 31.138 | 15.942 | 1.000 | 33.79 |
| ATOM | 2366 | O1 | HOH | W | 29 | 14.372  | 4.995  | 27.900 | 1.000 | 26.39 |
| ATOM | 2367 | O1 | HOH | W | 30 | -2.960  | 34.484 | 1.831  | 1.000 | 27.40 |
| ATOM | 2368 | O1 | HOH | W | 31 | 10.824  | 30.078 | 18.289 | 1.000 | 25.67 |
| ATOM | 2369 | O1 | HOH | W | 32 | 13.982  | 2.205  | 27.167 | 1.000 | 25.41 |
| ATOM | 2370 | O1 | HOH | W | 33 | 1.575   | 12.107 | 33.860 | 1.000 | 34.16 |
| ATOM | 2371 | O1 | HOH | W | 34 | -3.137  | 19.220 | -7.395 | 1.000 | 25.27 |
| ATOM | 2372 | O1 | HOH | W | 35 | -6.170  | 33.272 | 20.828 | 1.000 | 21.49 |
| ATOM | 2373 | O1 | HOH | W | 36 | -1.632  | 39.007 | 16.222 | 1.000 | 27.21 |
| ATOM | 2374 | O1 | HOH | W | 37 | 7.347   | 31.206 | 19.263 | 1.000 | 26.77 |
| ATOM | 2375 | O1 | HOH | W | 38 | 9.444   | 26.520 | 21.341 | 1.000 | 29.37 |
| ATOM | 2376 | O1 | HOH | W | 39 | -8.237  | 9.947  | 35.385 | 1.000 | 47.49 |
| ATOM | 2377 | O1 | HOH | W | 40 | -2.103  | 38.773 | 20.445 | 1.000 | 27.92 |
| ATOM | 2378 | O1 | HOH | W | 41 | -9.820  | 28.498 | 38.052 | 1.000 | 26.65 |
| ATOM | 2379 | O1 | HOH | W | 42 | 10.051  | 20.936 | -0.828 | 1.000 | 26.93 |
| ATOM | 2380 | O1 | HOH | W | 43 | -14.963 | 17.351 | 10.401 | 1.000 | 37.99 |
| ATOM | 2381 | O1 | HOH | W | 44 | 15.436  | 8.322  | 21.787 | 1.000 | 29.21 |
| ATOM | 2382 | O1 | HOH | W | 45 | 1.871   | 19.354 | 1.571  | 1.000 | 22.03 |
| ATOM | 2383 | O1 | HOH | W | 46 | -7.599  | 19.535 | 29.453 | 1.000 | 22.96 |
| ATOM | 2384 | O1 | HOH | W | 47 | 3.330   | 17.045 | 1.103  | 1.000 | 26.08 |
| ATOM | 2385 | O1 | HOH | W | 48 | 14.921  | 28.549 | 0.827  | 1.000 | 30.69 |
| ATOM | 2386 | O1 | HOH | W | 49 | 4.221   | 11.439 | 33.921 | 1.000 | 28.27 |
| ATOM | 2387 | O1 | HOH | W | 50 | 6.471   | 7.214  | 33.313 | 1.000 | 30.73 |
| ATOM | 2388 | O1 | HOH | W | 51 | 6.997   | 11.081 | 3.016  | 1.000 | 29.06 |
| ATOM | 2389 | O1 | HOH | W | 52 | 9.828   | 14.413 | 1.356  | 1.000 | 36.16 |
| ATOM | 2390 | O1 | HOH | W | 53 | -2.049  | 5.578  | 31.420 | 1.000 | 34.40 |
| ATOM | 2391 | O1 | HOH | W | 54 | 7.546   | 28.605 | 19.653 | 1.000 | 38.00 |

**FIGURE 247**

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Three Dimensional Coordinates of HPTPbeta

|      |      |    |     |   |     |         |        |        |       |       |
|------|------|----|-----|---|-----|---------|--------|--------|-------|-------|
| ATOM | 2392 | O1 | HOH | W | 55  | -11.689 | 15.787 | 24.708 | 1.000 | 27.99 |
| ATOM | 2393 | O1 | HOH | W | 56  | -1.930  | 38.222 | 3.832  | 1.000 | 26.57 |
| ATOM | 2394 | O1 | HOH | W | 57  | 3.629   | 5.858  | 35.758 | 1.000 | 33.41 |
| ATOM | 2395 | O1 | HOH | W | 58  | 2.994   | 20.770 | -0.697 | 1.000 | 26.75 |
| ATOM | 2396 | O1 | HOH | W | 59  | -13.363 | 22.643 | 29.523 | 1.000 | 32.53 |
| ATOM | 2397 | O1 | HOH | W | 60  | -3.967  | 36.098 | 3.552  | 1.000 | 24.24 |
| ATOM | 2398 | O1 | HOH | W | 61  | -13.003 | 28.717 | 20.098 | 1.000 | 30.30 |
| ATOM | 2399 | O1 | HOH | W | 62  | -3.571  | 34.737 | 21.021 | 1.000 | 24.77 |
| ATOM | 2400 | O1 | HOH | W | 63  | -3.353  | 25.782 | 37.784 | 1.000 | 31.16 |
| ATOM | 2401 | O1 | HOH | W | 64  | -4.181  | 15.085 | 11.174 | 1.000 | 23.09 |
| ATOM | 2402 | O1 | HOH | W | 65  | 14.882  | 1.430  | 29.740 | 1.000 | 32.36 |
| ATOM | 2403 | O1 | HOH | W | 66  | -2.385  | 10.919 | 14.099 | 1.000 | 31.04 |
| ATOM | 2404 | O1 | HOH | W | 67  | -2.022  | 11.997 | 12.100 | 1.000 | 34.23 |
| ATOM | 2405 | O1 | HOH | W | 68  | -0.074  | 6.701  | 29.852 | 1.000 | 28.84 |
| ATOM | 2406 | O1 | HOH | W | 69  | 13.012  | 17.319 | 31.049 | 1.000 | 34.35 |
| ATOM | 2407 | O1 | HOH | W | 70  | -0.945  | -1.322 | 32.490 | 1.000 | 27.87 |
| ATOM | 2408 | O1 | HOH | W | 71  | -14.687 | 16.999 | 7.638  | 1.000 | 39.15 |
| ATOM | 2409 | O1 | HOH | W | 72  | 5.621   | 40.002 | 16.979 | 1.000 | 36.19 |
| ATOM | 2410 | O1 | HOH | W | 73  | 5.019   | 34.934 | -5.124 | 1.000 | 30.14 |
| ATOM | 2411 | O1 | HOH | W | 74  | -13.469 | 20.866 | 21.275 | 1.000 | 35.79 |
| ATOM | 2412 | O1 | HOH | W | 75  | -6.587  | 38.439 | -4.937 | 1.000 | 34.64 |
| ATOM | 2413 | O1 | HOH | W | 76  | -6.586  | 20.943 | 1.389  | 1.000 | 34.28 |
| ATOM | 2414 | O1 | HOH | W | 77  | 16.678  | 2.326  | 14.116 | 1.000 | 34.62 |
| ATOM | 2415 | O1 | HOH | W | 78  | -0.115  | 2.845  | 36.291 | 1.000 | 30.53 |
| ATOM | 2416 | O1 | HOH | W | 79  | -0.221  | 19.000 | -0.242 | 1.000 | 25.17 |
| ATOM | 2417 | O1 | HOH | W | 80  | 18.011  | 13.617 | 17.062 | 1.000 | 28.47 |
| ATOM | 2418 | O1 | HOH | W | 81  | 8.378   | 5.752  | 31.945 | 1.000 | 25.91 |
| ATOM | 2419 | O1 | HOH | W | 82  | -1.655  | 40.288 | 22.680 | 1.000 | 32.53 |
| ATOM | 2420 | O1 | HOH | W | 83  | 6.545   | 30.062 | 22.582 | 1.000 | 41.03 |
| ATOM | 2421 | O1 | HOH | W | 84  | 8.148   | 39.805 | 15.692 | 1.000 | 35.25 |
| ATOM | 2422 | O1 | HOH | W | 85  | -14.461 | 20.880 | 32.244 | 1.000 | 35.66 |
| ATOM | 2423 | O1 | HOH | W | 86  | 5.851   | 3.752  | 34.055 | 1.000 | 36.71 |
| ATOM | 2424 | O1 | HOH | W | 87  | -0.955  | 1.090  | 13.636 | 1.000 | 39.92 |
| ATOM | 2425 | O1 | HOH | W | 88  | 8.422   | 39.414 | -0.957 | 1.000 | 48.27 |
| ATOM | 2426 | O1 | HOH | W | 89  | 10.954  | 39.318 | 2.465  | 1.000 | 44.33 |
| ATOM | 2427 | O1 | HOH | W | 90  | 2.579   | 50.503 | 2.300  | 1.000 | 54.86 |
| ATOM | 2428 | O1 | HOH | W | 91  | 3.085   | 48.432 | 3.786  | 1.000 | 37.84 |
| ATOM | 2429 | O1 | HOH | W | 92  | 6.015   | 47.673 | 10.758 | 1.000 | 46.93 |
| ATOM | 2430 | O1 | HOH | W | 93  | -4.388  | -7.612 | 19.050 | 1.000 | 45.59 |
| ATOM | 2431 | O1 | HOH | W | 94  | 0.214   | 18.775 | 39.716 | 1.000 | 51.95 |
| ATOM | 2432 | O1 | HOH | W | 95  | -12.966 | 13.296 | 30.655 | 1.000 | 33.33 |
| ATOM | 2433 | O1 | HOH | W | 96  | 0.538   | 14.855 | 35.881 | 1.000 | 40.77 |
| ATOM | 2434 | O1 | HOH | W | 97  | 17.070  | 25.109 | 3.747  | 1.000 | 45.67 |
| ATOM | 2435 | O1 | HOH | W | 98  | 11.830  | 27.957 | -0.458 | 1.000 | 43.72 |
| ATOM | 2436 | O1 | HOH | W | 99  | -4.616  | 12.312 | 11.217 | 1.000 | 40.90 |
| ATOM | 2437 | O1 | HOH | W | 100 | 11.872  | 35.092 | 7.761  | 1.000 | 55.45 |
| ATOM | 2438 | O1 | HOH | W | 101 | 10.663  | 36.578 | 9.005  | 1.000 | 38.01 |
| ATOM | 2439 | O1 | HOH | W | 102 | 14.787  | 30.925 | 2.347  | 1.000 | 38.58 |
| ATOM | 2440 | O1 | HOH | W | 103 | -7.639  | 22.432 | -0.126 | 1.000 | 30.65 |
| ATOM | 2441 | O1 | HOH | W | 104 | -0.768  | 39.758 | 18.325 | 1.000 | 32.85 |
| ATOM | 2442 | O1 | HOH | W | 105 | 11.805  | 25.356 | 22.168 | 1.000 | 40.43 |
| ATOM | 2443 | O1 | HOH | W | 106 | 20.422  | 18.338 | 13.902 | 1.000 | 45.59 |

**FIGURE 248**

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|      |      |    |           |         |        |        |       |        |
|------|------|----|-----------|---------|--------|--------|-------|--------|
| ATOM | 2444 | O1 | HOH W 107 | 10.183  | 24.874 | 30.453 | 1.000 | 38.68  |
| ATOM | 2445 | O1 | HOH W 108 | 16.785  | 32.728 | 12.612 | 1.000 | 31.96  |
| ATOM | 2446 | O1 | HOH W 109 | 13.492  | 30.752 | 17.655 | 1.000 | 39.37  |
| ATOM | 2447 | O1 | HOH W 110 | -3.931  | 16.862 | 2.029  | 1.000 | 30.36  |
| ATOM | 2448 | O1 | HOH W 111 | -7.045  | 29.232 | 5.340  | 1.000 | 28.48  |
| ATOM | 2449 | O1 | HOH W 112 | -7.762  | 11.786 | 25.923 | 1.000 | 28.04  |
| ATOM | 2450 | O1 | HOH W 113 | -13.605 | 33.677 | 20.128 | 1.000 | 32.20  |
| ATOM | 2451 | O1 | HOH W 114 | 10.065  | 39.638 | 9.803  | 1.000 | 38.13  |
| ATOM | 2452 | O1 | HOH W 115 | -8.934  | 24.435 | 1.974  | 1.000 | 31.50  |
| ATOM | 2453 | O1 | HOH W 116 | 17.216  | 10.741 | 21.573 | 1.000 | 34.76  |
| ATOM | 2454 | O1 | HOH W 117 | -11.923 | 22.839 | 19.220 | 1.000 | 39.73  |
| ATOM | 2455 | O1 | HOH W 118 | 7.473   | 12.705 | 1.120  | 1.000 | 36.05  |
| ATOM | 2456 | O1 | HOH W 119 | 5.483   | 8.873  | 2.549  | 1.000 | 43.08  |
| ATOM | 2457 | O1 | HOH W 120 | -14.010 | 13.235 | 28.254 | 1.000 | 43.67  |
| ATOM | 2458 | O1 | HOH W 121 | -6.810  | 4.829  | 28.513 | 1.000 | 38.61  |
| ATOM | 2459 | O1 | HOH W 122 | -14.132 | 10.542 | 31.339 | 1.000 | 58.03  |
| ATOM | 2460 | O1 | HOH W 123 | 5.390   | 21.831 | 37.038 | 1.000 | 43.01  |
| ATOM | 2461 | O1 | HOH W 124 | -14.479 | 21.966 | 26.038 | 1.000 | 35.30  |
| ATOM | 2462 | O1 | HOH W 125 | 4.264   | 17.945 | -1.288 | 1.000 | 36.29  |
| ATOM | 2463 | O1 | HOH W 126 | 23.828  | 24.174 | 30.873 | 1.000 | 49.73  |
| ATOM | 2464 | O1 | HOH W 127 | -6.176  | 26.450 | 5.939  | 1.000 | 65.00  |
| ATOM | 2465 | O1 | HOH W 128 | 3.350   | 34.622 | 26.589 | 1.000 | 39.90  |
| ATOM | 2466 | O1 | HOH W 129 | 16.916  | 27.171 | 7.485  | 1.000 | 41.94  |
| ATOM | 2467 | O1 | HOH W 130 | -11.189 | 32.210 | 8.814  | 1.000 | 35.24  |
| ATOM | 2468 | O1 | HOH W 131 | -4.460  | 2.050  | 29.021 | 1.000 | 40.95  |
| ATOM | 2469 | O1 | HOH W 132 | -15.621 | 16.785 | 16.397 | 1.000 | 51.14  |
| ATOM | 2470 | O1 | HOH W 133 | 13.141  | -0.750 | 30.285 | 1.000 | 35.50  |
| ATOM | 2471 | O1 | HOH W 134 | 16.391  | 14.131 | 18.996 | 1.000 | 33.72  |
| ATOM | 2472 | O1 | HOH W 135 | 15.720  | 23.607 | 18.037 | 1.000 | 36.32  |
| ATOM | 2473 | O1 | HOH W 136 | -9.180  | 28.989 | 7.435  | 1.000 | 51.57  |
| ATOM | 2474 | O1 | HOH W 137 | -13.398 | 18.098 | 35.125 | 1.000 | 52.51  |
| ATOM | 2475 | O1 | HOH W 138 | -14.347 | 26.998 | 19.051 | 1.000 | 43.88  |
| ATOM | 2476 | O1 | HOH W 139 | 17.167  | 1.215  | 28.662 | 1.000 | 40.00  |
| ATOM | 2477 | O1 | HOH W 140 | -5.468  | 13.807 | 7.111  | 1.000 | 45.45  |
| ATOM | 2478 | O1 | HOH W 141 | -4.475  | 4.635  | 29.841 | 1.000 | 36.10  |
| ATOM | 2479 | O1 | HOH W 142 | -12.828 | 27.385 | 13.802 | 1.000 | 33.50  |
| ATOM | 2480 | O1 | HOH W 143 | -13.938 | 17.712 | 24.521 | 1.000 | 31.09  |
| ATOM | 2481 | O1 | HOH W 144 | 16.503  | 26.254 | 10.447 | 1.000 | 46.13  |
| ATOM | 2482 | O1 | HOH W 145 | 20.599  | 20.875 | 15.821 | 1.000 | 41.98  |
| ATOM | 2483 | O1 | HOH W 146 | 20.503  | 19.870 | 22.082 | 1.000 | 51.04  |
| ATOM | 2484 | O1 | HOH W 147 | 4.262   | 18.175 | 36.175 | 1.000 | 33.32  |
| ATOM | 2485 | O1 | HOH W 148 | -0.297  | 26.441 | 36.081 | 1.000 | 52.28  |
| ATOM | 2486 | O1 | HOH W 149 | 20.297  | 28.737 | 16.671 | 1.000 | 44.74  |
| ATOM | 2487 | O1 | HOH W 150 | 7.203   | 23.388 | 35.762 | 1.000 | 66.45  |
| ATOM | 2488 | O1 | HOH W 151 | 10.549  | 7.398  | 31.284 | 1.000 | 38.68  |
| ATOM | 2489 | O1 | HOH W 152 | 6.081   | 38.872 | -2.812 | 1.000 | 40.08  |
| ATOM | 2490 | O1 | HOH W 153 | 13.265  | 33.000 | 1.040  | 1.000 | 36.24  |
| ATOM | 2491 | O1 | HOH W 154 | -12.530 | 39.835 | 27.125 | 1.000 | 105.41 |
| ATOM | 2492 | O1 | HOH W 155 | 11.420  | 11.430 | 30.533 | 1.000 | 47.78  |
| ATOM | 2493 | O1 | HOH W 156 | 0.901   | 8.244  | 35.852 | 1.000 | 33.14  |
| ATOM | 2494 | O1 | HOH W 157 | -7.963  | 29.336 | -0.295 | 1.000 | 50.61  |
| ATOM | 2495 | O1 | HOH W 158 | 20.035  | 12.009 | 18.471 | 1.000 | 34.37  |

**FIGURE 249**

|      |      |    |           |         |        |         |       |       |
|------|------|----|-----------|---------|--------|---------|-------|-------|
| ATOM | 2496 | O1 | HOH W 159 | -4.350  | 3.543  | 10.491  | 1.000 | 84.51 |
| ATOM | 2497 | O1 | HOH W 160 | 4.286   | 9.674  | 36.102  | 1.000 | 40.87 |
| ATOM | 2498 | O1 | HOH W 161 | -8.003  | 41.353 | 17.020  | 1.000 | 48.97 |
| ATOM | 2499 | O1 | HOH W 162 | 15.195  | 17.562 | 28.763  | 1.000 | 43.23 |
| ATOM | 2500 | O1 | HOH W 163 | -10.778 | 5.540  | 28.103  | 1.000 | 47.36 |
| ATOM | 2501 | O1 | HOH W 164 | 19.303  | 31.924 | 16.796  | 1.000 | 51.07 |
| ATOM | 2502 | O1 | HOH W 165 | -4.383  | 19.665 | -0.828  | 1.000 | 32.47 |
| ATOM | 2503 | O1 | HOH W 166 | 8.839   | 24.816 | -3.783  | 1.000 | 41.71 |
| ATOM | 2504 | O1 | HOH W 167 | 6.219   | 15.861 | -1.300  | 1.000 | 43.10 |
| ATOM | 2505 | O1 | HOH W 168 | 10.025  | 33.624 | 18.562  | 1.000 | 40.32 |
| ATOM | 2506 | O1 | HOH W 169 | 7.836   | 30.797 | 27.712  | 1.000 | 56.16 |
| ATOM | 2507 | O1 | HOH W 170 | -9.946  | 19.362 | 35.362  | 1.000 | 41.05 |
| ATOM | 2508 | O1 | HOH W 171 | 22.397  | 23.179 | 24.094  | 1.000 | 37.17 |
| ATOM | 2509 | O1 | HOH W 172 | 6.196   | 31.438 | 24.998  | 1.000 | 39.04 |
| ATOM | 2510 | O1 | HOH W 173 | 2.656   | 29.647 | -11.398 | 1.000 | 69.02 |
| ATOM | 2511 | O1 | HOH W 174 | -7.993  | 19.195 | 2.017   | 1.000 | 51.50 |
| ATOM | 2512 | O1 | HOH W 175 | -7.725  | 9.838  | 10.116  | 1.000 | 41.23 |
| ATOM | 2513 | O1 | HOH W 176 | 10.217  | 8.209  | 35.322  | 1.000 | 52.55 |
| ATOM | 2514 | O1 | HOH W 177 | 22.886  | 18.048 | 5.069   | 1.000 | 50.22 |
| ATOM | 2515 | O1 | HOH W 178 | 13.259  | 6.843  | 29.204  | 1.000 | 37.28 |
| ATOM | 2516 | O1 | HOH W 179 | -11.344 | 39.086 | 20.797  | 1.000 | 63.58 |
| ATOM | 2517 | O1 | HOH W 180 | 13.661  | 33.712 | 7.349   | 1.000 | 48.08 |
| ATOM | 2518 | O1 | HOH W 181 | -3.554  | 0.841  | 36.601  | 1.000 | 44.25 |
| ATOM | 2519 | O1 | HOH W 182 | 2.483   | 16.905 | 37.338  | 1.000 | 45.30 |
| ATOM | 2520 | O1 | HOH W 183 | 20.094  | 7.002  | 12.783  | 1.000 | 44.53 |
| ATOM | 2521 | O1 | HOH W 184 | 13.549  | 19.866 | -1.559  | 1.000 | 51.39 |
| ATOM | 2522 | O1 | HOH W 185 | 11.649  | -2.468 | 19.869  | 1.000 | 58.70 |
| ATOM | 2523 | O1 | HOH W 186 | -11.387 | 9.057  | 20.869  | 1.000 | 50.26 |
| ATOM | 2524 | O1 | HOH W 187 | 2.270   | 53.746 | 3.948   | 1.000 | 77.69 |
| ATOM | 2525 | O1 | HOH W 188 | 7.272   | 43.089 | 10.416  | 1.000 | 40.06 |
| ATOM | 2526 | O1 | HOH W 189 | -10.704 | 43.630 | 20.531  | 1.000 | 67.96 |
| ATOM | 2527 | O1 | HOH W 190 | -10.161 | 31.212 | -6.317  | 1.000 | 49.46 |
| ATOM | 2528 | O1 | HOH W 191 | 9.522   | 6.064  | 4.334   | 1.000 | 40.34 |
| ATOM | 2529 | O1 | HOH W 192 | 16.516  | 16.717 | 21.174  | 1.000 | 20.43 |
| ATOM | 2530 | O1 | HOH W 193 | -0.857  | 36.253 | 20.284  | 1.000 | 32.45 |
| ATOM | 2531 | O1 | HOH W 194 | 18.504  | 18.275 | 22.970  | 1.000 | 34.08 |
| ATOM | 2532 | O1 | HOH W 195 | 5.801   | 29.116 | -17.383 | 1.000 | 43.44 |
| ATOM | 2533 | O1 | HOH W 196 | -7.990  | 22.703 | 42.079  | 1.000 | 44.28 |
| ATOM | 2534 | O1 | HOH W 197 | -6.632  | 16.747 | 36.401  | 1.000 | 37.74 |
| ATOM | 2535 | O1 | HOH W 198 | -11.815 | 21.607 | 16.468  | 1.000 | 30.66 |
| ATOM | 2536 | O1 | HOH W 199 | -2.843  | 32.478 | -11.634 | 1.000 | 33.04 |
| ATOM | 2537 | O1 | HOH W 200 | -10.429 | 21.931 | 2.610   | 1.000 | 43.58 |
| ATOM | 2538 | O1 | HOH W 201 | -12.782 | 11.466 | 36.315  | 1.000 | 64.73 |
| ATOM | 2539 | O1 | HOH W 202 | -1.120  | 8.730  | 9.515   | 1.000 | 39.25 |
| ATOM | 2540 | O1 | HOH W 203 | 7.752   | 27.565 | 23.146  | 1.000 | 40.81 |
| ATOM | 2541 | O1 | HOH W 204 | -4.173  | 17.946 | -3.218  | 1.000 | 40.93 |
| ATOM | 2542 | O1 | HOH W 205 | -12.084 | 5.496  | 19.653  | 1.000 | 41.61 |
| ATOM | 2543 | O1 | HOH W 206 | 1.514   | 0.000  | 33.985  | 1.000 | 47.99 |
| ATOM | 2544 | O1 | HOH W 207 | -4.358  | 32.825 | -9.953  | 1.000 | 43.82 |
| ATOM | 2545 | O1 | HOH W 208 | 14.414  | 14.005 | 29.829  | 1.000 | 45.03 |
| ATOM | 2546 | O1 | HOH W 209 | 22.352  | 27.139 | 21.459  | 1.000 | 63.00 |
| ATOM | 2547 | O1 | HOH W 210 | -12.128 | 21.274 | 9.705   | 1.000 | 39.35 |

**FIGURE 250**

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|      |      |    |           |         |        |         |       |       |
|------|------|----|-----------|---------|--------|---------|-------|-------|
| ATOM | 2548 | O1 | HOH W 211 | -15.431 | 29.589 | 23.297  | 1.000 | 42.10 |
| ATOM | 2549 | O1 | HOH W 212 | 15.717  | 21.134 | 2.051   | 1.000 | 44.92 |
| ATOM | 2550 | O1 | HOH W 213 | 22.149  | 19.371 | 9.989   | 1.000 | 42.03 |
| ATOM | 2551 | O1 | HOH W 214 | -12.478 | 28.555 | 38.340  | 1.000 | 49.23 |
| ATOM | 2552 | O1 | HOH W 215 | -10.373 | 26.583 | 11.557  | 1.000 | 78.42 |
| ATOM | 2553 | O1 | HOH W 216 | 5.904   | 28.076 | 21.168  | 1.000 | 47.47 |
| ATOM | 2554 | O1 | HOH W 217 | 18.063  | 28.353 | 10.622  | 1.000 | 39.47 |
| ATOM | 2555 | O1 | HOH W 218 | 5.741   | 29.596 | 34.757  | 1.000 | 50.24 |
| ATOM | 2556 | O1 | HOH W 219 | 23.482  | 28.211 | 28.256  | 1.000 | 35.92 |
| ATOM | 2557 | O1 | HOH W 220 | 20.729  | 22.839 | 22.289  | 1.000 | 47.92 |
| ATOM | 2558 | O1 | HOH W 221 | -13.743 | 23.631 | 15.768  | 1.000 | 56.18 |
| ATOM | 2559 | O1 | HOH W 222 | 0.808   | 4.763  | 11.965  | 1.000 | 52.58 |
| ATOM | 2560 | O1 | HOH W 223 | 19.695  | 26.083 | 30.808  | 1.000 | 48.34 |
| ATOM | 2561 | O1 | HOH W 224 | -10.086 | 39.766 | 26.571  | 1.000 | 37.07 |
| ATOM | 2562 | O1 | HOH W 225 | -8.185  | 26.002 | 12.785  | 1.000 | 43.04 |
| ATOM | 2563 | O1 | HOH W 226 | -15.767 | 14.896 | 27.476  | 1.000 | 47.84 |
| ATOM | 2564 | O1 | HOH W 227 | -8.943  | 41.210 | 23.852  | 1.000 | 51.44 |
| ATOM | 2565 | O1 | HOH W 228 | -13.243 | 38.293 | 6.326   | 1.000 | 46.48 |
| ATOM | 2566 | O1 | HOH W 229 | 18.663  | 0.325  | 20.946  | 1.000 | 45.85 |
| ATOM | 2567 | O1 | HOH W 230 | 12.773  | 6.887  | 31.536  | 1.000 | 35.71 |
| ATOM | 2568 | O1 | HOH W 231 | -7.081  | 32.709 | -9.020  | 1.000 | 54.13 |
| ATOM | 2569 | O1 | HOH W 232 | -14.685 | 24.271 | 19.574  | 1.000 | 44.68 |
| ATOM | 2570 | O1 | HOH W 233 | 1.541   | 7.037  | 10.861  | 1.000 | 42.37 |
| ATOM | 2571 | O1 | HOH W 234 | 17.407  | 14.624 | 24.034  | 1.000 | 49.34 |
| ATOM | 2572 | O1 | HOH W 235 | -8.898  | 25.154 | 4.255   | 1.000 | 55.39 |
| ATOM | 2573 | O1 | HOH W 236 | 9.061   | 28.544 | 24.947  | 1.000 | 39.46 |
| ATOM | 2574 | O1 | HOH W 237 | -13.663 | 15.439 | 32.214  | 1.000 | 45.65 |
| ATOM | 2575 | O1 | HOH W 238 | 13.791  | 17.581 | 34.085  | 1.000 | 46.31 |
| ATOM | 2576 | O1 | HOH W 239 | -11.961 | 16.055 | 13.445  | 1.000 | 40.48 |
| ATOM | 2577 | O1 | HOH W 240 | 15.223  | 9.544  | 28.176  | 1.000 | 44.69 |
| ATOM | 2578 | O1 | HOH W 241 | -13.353 | 32.529 | 7.227   | 1.000 | 57.27 |
| ATOM | 2579 | O1 | HOH W 242 | 8.996   | 26.371 | -16.754 | 1.000 | 48.64 |
| ATOM | 2580 | O1 | HOH W 243 | 6.092   | 23.068 | -5.367  | 1.000 | 48.87 |
| ATOM | 2581 | O1 | HOH W 244 | 22.747  | 32.593 | 25.452  | 1.000 | 44.40 |
| ATOM | 2582 | O1 | HOH W 245 | -0.304  | 32.548 | -11.298 | 1.000 | 48.96 |
| ATOM | 2583 | O1 | HOH W 246 | -4.988  | -3.152 | 23.809  | 1.000 | 62.34 |
| ATOM | 2584 | O1 | HOH W 247 | 1.129   | 39.597 | -7.798  | 1.000 | 53.14 |
| ATOM | 2585 | O1 | HOH W 248 | -6.772  | 14.727 | 4.405   | 1.000 | 81.57 |
| ATOM | 2586 | O1 | HOH W 249 | 17.223  | 10.068 | 27.178  | 1.000 | 40.37 |
| ATOM | 2587 | O1 | HOH W 250 | 17.655  | 12.530 | 28.719  | 1.000 | 50.20 |
| ATOM | 2588 | O1 | HOH W 251 | 4.037   | 7.351  | 8.012   | 1.000 | 58.42 |
| ATOM | 2589 | O1 | HOH W 252 | -1.828  | 7.240  | 33.526  | 1.000 | 45.82 |
| ATOM | 2590 | O1 | HOH W 253 | -12.257 | 12.014 | 23.313  | 1.000 | 42.52 |
| ATOM | 2591 | O1 | HOH W 254 | 18.878  | 30.723 | 23.928  | 1.000 | 81.96 |
| ATOM | 2592 | O1 | HOH W 255 | -2.406  | 13.001 | 35.608  | 1.000 | 49.36 |
| ATOM | 2593 | O1 | HOH W 256 | 0.100   | 42.639 | 18.634  | 1.000 | 42.69 |
| ATOM | 2594 | O1 | HOH W 257 | 8.781   | 15.841 | -0.776  | 1.000 | 42.10 |
| ATOM | 2595 | O1 | HOH W 258 | 8.836   | 41.627 | 14.232  | 1.000 | 37.51 |
| ATOM | 2596 | O1 | HOH W 259 | 10.082  | 41.227 | 7.652   | 1.000 | 51.86 |
| ATOM | 2597 | O1 | HOH W 260 | 16.536  | 4.886  | 29.969  | 1.000 | 46.99 |
| ATOM | 2598 | O1 | HOH W 261 | 8.904   | 2.996  | 11.102  | 1.000 | 59.35 |
| ATOM | 2599 | O1 | HOH W 262 | 17.169  | 18.558 | 5.383   | 1.000 | 42.46 |

**FIGURE 251**

|      |      |    |           |         |        |         |       |        |
|------|------|----|-----------|---------|--------|---------|-------|--------|
| ATOM | 2600 | O1 | HOH W 263 | 22.449  | 12.846 | 9.882   | 1.000 | 39.10  |
| ATOM | 2601 | O1 | HOH W 264 | 11.441  | 22.960 | -0.297  | 1.000 | 46.40  |
| ATOM | 2602 | O1 | HOH W 265 | 12.891  | 35.186 | -7.958  | 1.000 | 59.81  |
| ATOM | 2603 | O1 | HOH W 266 | -13.897 | 24.909 | 13.026  | 1.000 | 45.86  |
| ATOM | 2604 | O1 | HOH W 267 | 19.060  | 9.563  | 25.380  | 1.000 | 45.48  |
| ATOM | 2605 | O1 | HOH W 268 | 3.802   | 25.392 | -14.805 | 1.000 | 50.59  |
| ATOM | 2606 | O1 | HOH W 269 | 16.184  | 28.549 | 22.110  | 1.000 | 43.02  |
| ATOM | 2607 | O1 | HOH W 270 | -1.154  | 37.399 | -12.192 | 1.000 | 53.68  |
| ATOM | 2608 | O1 | HOH W 271 | -4.123  | -5.269 | 18.602  | 1.000 | 79.29  |
| ATOM | 2609 | O1 | HOH W 272 | -7.384  | 2.425  | 21.048  | 1.000 | 57.48  |
| ATOM | 2610 | O1 | HOH W 273 | 18.456  | 25.557 | 18.479  | 1.000 | 44.20  |
| ATOM | 2611 | O1 | HOH W 274 | 6.328   | 1.205  | 9.458   | 1.000 | 59.21  |
| ATOM | 2612 | O1 | HOH W 275 | -14.117 | 5.491  | 34.696  | 1.000 | 60.85  |
| ATOM | 2613 | O1 | HOH W 276 | -10.629 | 13.583 | 38.737  | 1.000 | 45.87  |
| ATOM | 2614 | O1 | HOH W 277 | -11.913 | 20.085 | 36.715  | 1.000 | 51.46  |
| ATOM | 2615 | O1 | HOH W 278 | -8.375  | 43.387 | 4.147   | 1.000 | 45.52  |
| ATOM | 2616 | O1 | HOH W 279 | -9.702  | -4.797 | 28.731  | 1.000 | 54.85  |
| ATOM | 2617 | O1 | HOH W 280 | -12.340 | 25.454 | 10.801  | 1.000 | 58.08  |
| ATOM | 2618 | O1 | HOH W 281 | -4.825  | 10.727 | 8.928   | 1.000 | 55.18  |
| ATOM | 2619 | O1 | HOH W 282 | -0.469  | 27.271 | 21.450  | 1.000 | 143.86 |
| ATOM | 2620 | O1 | HOH W 283 | 1.342   | 6.223  | -2.164  | 1.000 | 59.20  |
| ATOM | 2621 | O1 | HOH W 284 | -13.187 | 3.566  | 20.610  | 1.000 | 59.09  |
| ATOM | 2622 | O1 | HOH W 285 | -10.963 | -4.464 | 24.556  | 1.000 | 70.44  |
| ATOM | 2623 | O1 | HOH W 286 | 2.082   | 7.263  | 5.127   | 1.000 | 59.07  |
| ATOM | 2624 | O1 | HOH W 287 | -14.375 | 31.030 | 19.349  | 1.000 | 42.90  |
| ATOM | 2625 | O1 | HOH W 288 | -13.932 | 23.344 | 10.653  | 1.000 | 42.75  |
| ATOM | 2626 | O1 | HOH W 289 | -10.496 | 31.449 | 2.357   | 1.000 | 37.15  |
| ATOM | 2627 | O1 | HOH W 290 | -5.935  | 42.393 | 1.278   | 1.000 | 48.92  |
| ATOM | 2628 | O1 | HOH W 291 | -2.417  | 29.064 | 38.937  | 1.000 | 98.13  |
| ATOM | 2629 | O1 | HOH W 292 | 4.370   | 7.161  | 3.591   | 1.000 | 54.78  |
| ATOM | 2630 | O1 | HOH W 293 | -12.101 | 29.567 | -1.765  | 1.000 | 45.21  |
| ATOM | 2631 | O1 | HOH W 294 | -2.974  | 52.167 | 6.924   | 1.000 | 54.46  |
| ATOM | 2632 | O1 | HOH W 295 | 6.373   | 24.732 | -15.736 | 1.000 | 55.54  |
| ATOM | 2633 | O1 | HOH W 296 | 5.144   | 2.212  | 15.505  | 1.000 | 132.19 |
| ATOM | 2634 | O1 | HOH W 297 | 4.119   | 25.540 | -18.043 | 1.000 | 63.04  |
| ATOM | 2635 | O1 | HOH W 298 | -6.584  | 46.120 | 5.004   | 1.000 | 61.91  |
| ATOM | 2636 | O1 | HOH W 299 | 17.182  | 15.542 | 27.047  | 1.000 | 45.04  |
| ATOM | 2637 | O1 | HOH W 300 | 12.276  | 33.194 | -3.953  | 1.000 | 50.26  |
| ATOM | 2638 | O1 | HOH W 301 | 4.057   | 25.805 | 36.737  | 1.000 | 51.03  |
| ATOM | 2639 | O1 | HOH W 302 | 17.210  | 27.508 | 26.182  | 1.000 | 43.16  |
| ATOM | 2640 | O1 | HOH W 303 | -13.383 | 20.836 | 7.055   | 1.000 | 53.40  |
| ATOM | 2641 | O1 | HOH W 304 | 19.482  | 17.276 | 28.478  | 1.000 | 60.44  |
| ATOM | 2642 | O1 | HOH W 305 | -6.950  | 41.249 | -1.159  | 1.000 | 53.64  |
| ATOM | 2643 | O1 | HOH W 306 | -10.165 | 8.508  | 39.743  | 1.000 | 61.15  |
| ATOM | 2644 | O1 | HOH W 307 | 4.134   | 19.769 | -3.502  | 1.000 | 52.25  |
| ATOM | 2645 | O1 | HOH W 308 | 3.101   | 15.563 | -2.031  | 1.000 | 45.06  |
| ATOM | 2646 | O1 | HOH W 309 | 8.724   | 40.739 | 11.753  | 1.000 | 47.08  |
| ATOM | 2647 | O1 | HOH W 310 | -10.535 | 2.414  | 25.587  | 1.000 | 88.70  |
| END  |      |    |           |         |        |         |       |        |

**FIGURE 252**



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|        |        |        |           |         |        |         |            |
|--------|--------|--------|-----------|---------|--------|---------|------------|
| CRYST1 | 38.852 | 69.610 | 117.777   | 90.00   | 90.00  | 90.00   | P 21 21 21 |
| ATOM   | 1      | N      | LYS A 19  | -13.362 | 32.383 | 10.240  | 1.00 48.36 |
| ATOM   | 2      | CA     | LYS A 19  | -13.935 | 33.412 | 9.318   | 1.00 47.56 |
| ATOM   | 3      | CB     | LYS A 19  | -14.789 | 34.414 | 10.102  | 1.00 48.40 |
| ATOM   | 4      | CG     | LYS A 19  | -16.107 | 34.813 | 9.444   | 1.00 50.42 |
| ATOM   | 5      | CD     | LYS A 19  | -16.509 | 36.212 | 9.896   | 1.00 51.36 |
| ATOM   | 6      | CE     | LYS A 19  | -17.815 | 36.655 | 9.263   | 1.00 52.93 |
| ATOM   | 7      | NZ     | LYS A 19  | -18.963 | 36.009 | 9.969   | 1.00 50.02 |
| ATOM   | 8      | C      | LYS A 19  | -12.885 | 34.153 | 8.487   | 1.00 45.61 |
| ATOM   | 9      | O      | LYS A 19  | -12.823 | 33.994 | 7.265   | 1.00 46.13 |
| ATOM   | 10     | N      | THR A 20  | -12.070 | 34.966 | 9.153   | 1.00 43.56 |
| ATOM   | 11     | CA     | THR A 20  | -11.312 | 35.995 | 8.460   | 1.00 40.00 |
| ATOM   | 12     | CB     | THR A 20  | -11.081 | 37.248 | 9.348   | 1.00 41.25 |
| ATOM   | 13     | OG1    | THR A 20  | -11.320 | 38.444 | 8.598   | 1.00 41.63 |
| ATOM   | 14     | CG2    | THR A 20  | -9.647  | 37.393 | 9.810   | 1.00 43.82 |
| ATOM   | 15     | C      | THR A 20  | -10.091 | 35.385 | 7.764   | 1.00 36.65 |
| ATOM   | 16     | O      | THR A 20  | -9.557  | 34.349 | 8.149   | 1.00 34.08 |
| ATOM   | 17     | N      | SER A 21  | -9.707  | 36.004 | 6.662   | 1.00 33.82 |
| ATOM   | 18     | CA     | SER A 21  | -9.158  | 35.238 | 5.553   | 1.00 31.39 |
| ATOM   | 19     | CB     | SER A 21  | -10.279 | 34.427 | 4.900   | 1.00 32.67 |
| ATOM   | 20     | OG     | SER A 21  | -9.913  | 33.919 | 3.630   | 1.00 34.27 |
| ATOM   | 21     | C      | SER A 21  | -8.654  | 36.302 | 4.606   | 1.00 31.16 |
| ATOM   | 22     | O      | SER A 21  | -9.312  | 37.328 | 4.434   | 1.00 30.44 |
| ATOM   | 23     | N      | CYS A 22  | -7.494  | 36.064 | 4.005   | 1.00 28.46 |
| ATOM   | 24     | CA     | CYS A 22  | -6.989  | 36.913 | 2.927   | 1.00 28.63 |
| ATOM   | 25     | CB     | CYS A 22  | -5.891  | 37.819 | 3.465   | 1.00 28.57 |
| ATOM   | 26     | SG     | ACYS A 22 | -6.413  | 38.961 | 4.757   | 0.50 34.99 |
| ATOM   | 27     | SG     | BCYS A 22 | -5.652  | 39.300 | 2.462   | 0.50 30.02 |
| ATOM   | 28     | C      | CYS A 22  | -6.377  | 36.077 | 1.801   | 1.00 26.91 |
| ATOM   | 29     | O      | CYS A 22  | -5.154  | 35.976 | 1.717   | 1.00 26.74 |
| ATOM   | 30     | N      | PRO A 23  | -7.204  | 35.459 | 0.965   | 1.00 27.39 |
| ATOM   | 31     | CA     | PRO A 23  | -6.683  | 34.571 | -0.080  | 1.00 27.48 |
| ATOM   | 32     | CB     | PRO A 23  | -7.934  | 33.853 | -0.574  | 1.00 28.38 |
| ATOM   | 33     | CG     | PRO A 23  | -8.993  | 34.875 | -0.368  | 1.00 30.20 |
| ATOM   | 34     | CD     | PRO A 23  | -8.674  | 35.517 | 0.952   | 1.00 27.17 |
| ATOM   | 35     | C      | PRO A 23  | -6.036  | 35.395 | -1.185  | 1.00 27.85 |
| ATOM   | 36     | O      | PRO A 23  | -6.513  | 36.495 | -1.487  | 1.00 28.68 |
| ATOM   | 37     | N      | ILE A 24  | -4.929  | 34.890 | -1.723  | 1.00 25.89 |
| ATOM   | 38     | CA     | ILE A 24  | -4.148  | 35.595 | -2.723  | 1.00 24.61 |
| ATOM   | 39     | CB     | ILE A 24  | -2.747  | 35.890 | -2.154  | 1.00 25.01 |
| ATOM   | 40     | CG1    | ILE A 24  | -2.821  | 36.742 | -0.873  | 1.00 23.94 |
| ATOM   | 41     | CD1    | ILE A 24  | -3.654  | 38.013 | -1.033  | 1.00 28.76 |
| ATOM   | 42     | CG2    | ILE A 24  | -1.845  | 36.467 | -3.229  | 1.00 24.43 |
| ATOM   | 43     | C      | ILE A 24  | -4.044  | 34.641 | -3.898  | 1.00 24.73 |
| ATOM   | 44     | O      | ILE A 24  | -3.774  | 33.445 | -3.719  | 1.00 24.14 |
| ATOM   | 45     | N      | LYS A 25  | -4.262  | 35.138 | -5.112  | 1.00 23.63 |
| ATOM   | 46     | CA     | LYS A 25  | -4.158  | 34.245 | -6.261  | 1.00 23.86 |
| ATOM   | 47     | CB     | LYS A 25  | -4.639  | 34.948 | -7.538  | 1.00 25.41 |
| ATOM   | 48     | CG     | LYS A 25  | -6.138  | 35.188 | -7.552  | 1.00 29.05 |
| ATOM   | 49     | CD     | LYS A 25  | -6.540  | 35.965 | -8.799  | 1.00 35.15 |
| ATOM   | 50     | CE     | LYS A 25  | -8.054  | 36.059 | -8.951  | 1.00 40.89 |
| ATOM   | 51     | NZ     | LYS A 25  | -8.390  | 36.581 | -10.313 | 1.00 45.05 |

**FIGURE 253**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |         |      |       |
|------|-----|-----|-----|---|----|--------|--------|---------|------|-------|
| ATOM | 52  | C   | LYS | A | 25 | -2.688 | 33.885 | -6.407  | 1.00 | 22.99 |
| ATOM | 53  | O   | LYS | A | 25 | -1.823 | 34.725 | -6.195  | 1.00 | 23.91 |
| ATOM | 54  | N   | ILE | A | 26 | -2.374 | 32.643 | -6.762  | 1.00 | 24.14 |
| ATOM | 55  | CA  | ILE | A | 26 | -0.961 | 32.283 | -6.723  | 1.00 | 26.45 |
| ATOM | 56  | CB  | ILE | A | 26 | -0.718 | 30.774 | -6.781  | 1.00 | 26.63 |
| ATOM | 57  | CG1 | ILE | A | 26 | -1.088 | 30.233 | -8.158  | 1.00 | 25.40 |
| ATOM | 58  | CD1 | ILE | A | 26 | -0.405 | 28.926 | -8.497  | 1.00 | 33.92 |
| ATOM | 59  | CG2 | ILE | A | 26 | -1.424 | 30.068 | -5.616  | 1.00 | 25.53 |
| ATOM | 60  | C   | ILE | A | 26 | -0.148 | 33.072 | -7.745  | 1.00 | 28.11 |
| ATOM | 61  | O   | ILE | A | 26 | 1.003  | 33.402 | -7.493  | 1.00 | 30.02 |
| ATOM | 62  | N   | ASN | A | 27 | -0.770 | 33.454 | -8.855  | 1.00 | 30.78 |
| ATOM | 63  | CA  | ASN | A | 27 | -0.033 | 34.223 | -9.862  | 1.00 | 35.08 |
| ATOM | 64  | CB  | ASN | A | 27 | -0.710 | 34.094 | -11.236 | 1.00 | 34.95 |
| ATOM | 65  | CG  | ASN | A | 27 | -1.552 | 32.824 | -11.347 | 1.00 | 40.82 |
| ATOM | 66  | OD1 | ASN | A | 27 | -1.093 | 31.822 | -11.915 | 1.00 | 44.00 |
| ATOM | 67  | ND2 | ASN | A | 27 | -2.770 | 32.844 | -10.778 | 1.00 | 42.15 |
| ATOM | 68  | C   | ASN | A | 27 | 0.174  | 35.683 | -9.455  | 1.00 | 34.87 |
| ATOM | 69  | O   | ASN | A | 27 | 0.938  | 36.415 | -10.098 | 1.00 | 38.32 |
| ATOM | 70  | N   | GLN | A | 28 | -0.491 | 36.100 | -8.379  | 1.00 | 33.79 |
| ATOM | 71  | CA  | GLN | A | 28 | -0.283 | 37.411 | -7.776  | 1.00 | 33.05 |
| ATOM | 72  | CB  | GLN | A | 28 | -1.633 | 38.093 | -7.546  | 1.00 | 34.54 |
| ATOM | 73  | CG  | GLN | A | 28 | -2.004 | 39.014 | -8.699  | 1.00 | 40.43 |
| ATOM | 74  | CD  | GLN | A | 28 | -3.422 | 38.827 | -9.172  | 1.00 | 46.19 |
| ATOM | 75  | OE1 | GLN | A | 28 | -4.339 | 38.673 | -8.362  | 1.00 | 49.62 |
| ATOM | 76  | NE2 | GLN | A | 28 | -3.612 | 38.845 | -10.491 | 1.00 | 49.01 |
| ATOM | 77  | C   | GLN | A | 28 | 0.520  | 37.409 | -6.478  | 1.00 | 31.93 |
| ATOM | 78  | O   | GLN | A | 28 | 0.823  | 38.469 | -5.920  | 1.00 | 30.78 |
| ATOM | 79  | N   | PHE | A | 29 | 0.863  | 36.216 | -5.996  | 1.00 | 31.01 |
| ATOM | 80  | CA  | PHE | A | 29 | 1.573  | 36.132 | -4.720  | 1.00 | 29.71 |
| ATOM | 81  | CB  | PHE | A | 29 | 1.805  | 34.688 | -4.249  | 1.00 | 29.10 |
| ATOM | 82  | CG  | PHE | A | 29 | 2.257  | 34.608 | -2.809  | 1.00 | 25.53 |
| ATOM | 83  | CD1 | PHE | A | 29 | 1.331  | 34.519 | -1.790  | 1.00 | 25.89 |
| ATOM | 84  | CE1 | PHE | A | 29 | 1.749  | 34.470 | -0.465  | 1.00 | 25.38 |
| ATOM | 85  | CZ  | PHE | A | 29 | 3.101  | 34.545 | -0.156  | 1.00 | 23.03 |
| ATOM | 86  | CE2 | PHE | A | 29 | 4.024  | 34.658 | -1.171  | 1.00 | 22.38 |
| ATOM | 87  | CD2 | PHE | A | 29 | 3.608  | 34.678 | -2.481  | 1.00 | 22.17 |
| ATOM | 88  | C   | PHE | A | 29 | 2.872  | 36.930 | -4.662  | 1.00 | 31.08 |
| ATOM | 89  | O   | PHE | A | 29 | 3.104  | 37.662 | -3.690  | 1.00 | 30.41 |
| ATOM | 90  | N   | GLU | A | 30 | 3.719  | 36.779 | -5.680  | 1.00 | 30.60 |
| ATOM | 91  | CA  | GLU | A | 30 | 5.044  | 37.388 | -5.633  | 1.00 | 32.65 |
| ATOM | 92  | CB  | GLU | A | 30 | 5.766  | 37.120 | -6.953  | 1.00 | 33.47 |
| ATOM | 93  | CG  | GLU | A | 30 | 7.107  | 37.828 | -7.096  | 1.00 | 38.26 |
| ATOM | 94  | CD  | GLU | A | 30 | 8.210  | 37.192 | -6.273  | 1.00 | 41.01 |
| ATOM | 95  | OE1 | GLU | A | 30 | 8.324  | 35.942 | -6.263  | 1.00 | 41.31 |
| ATOM | 96  | OE2 | GLU | A | 30 | 8.972  | 37.954 | -5.638  | 1.00 | 43.55 |
| ATOM | 97  | C   | GLU | A | 30 | 4.913  | 38.890 | -5.391  | 1.00 | 32.57 |
| ATOM | 98  | O   | GLU | A | 30 | 5.570  | 39.475 | -4.523  | 1.00 | 31.57 |
| ATOM | 99  | N   | GLY | A | 31 | 4.031  | 39.504 | -6.171  | 1.00 | 34.44 |
| ATOM | 100 | CA  | GLY | A | 31 | 3.688  | 40.905 | -5.986  | 1.00 | 35.40 |
| ATOM | 101 | C   | GLY | A | 31 | 2.984  | 41.274 | -4.697  | 1.00 | 35.45 |
| ATOM | 102 | O   | GLY | A | 31 | 3.285  | 42.311 | -4.102  | 1.00 | 36.66 |
| ATOM | 103 | N   | HIS | A | 32 | 2.040  | 40.449 | -4.250  | 1.00 | 35.17 |

**FIGURE 254**

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|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 104 | CA  | HIS | A | 32 | 1.406  | 40.666 | -2.953 | 1.00 | 34.19 |
| ATOM | 105 | CB  | HIS | A | 32 | 0.377  | 39.571 | -2.650 | 1.00 | 33.45 |
| ATOM | 106 | CG  | HIS | A | 32 | -0.137 | 39.576 | -1.239 | 1.00 | 35.35 |
| ATOM | 107 | ND1 | HIS | A | 32 | -1.005 | 40.533 | -0.759 | 1.00 | 34.86 |
| ATOM | 108 | CE1 | HIS | A | 32 | -1.294 | 40.275 | 0.504  | 1.00 | 38.34 |
| ATOM | 109 | NE2 | HIS | A | 32 | -0.667 | 39.165 | 0.856  | 1.00 | 39.21 |
| ATOM | 110 | CD2 | HIS | A | 32 | 0.072  | 38.714 | -0.212 | 1.00 | 36.26 |
| ATOM | 111 | C   | HIS | A | 32 | 2.471  | 40.749 | -1.861 | 1.00 | 33.35 |
| ATOM | 112 | O   | HIS | A | 32 | 2.461  | 41.663 | -1.037 | 1.00 | 31.23 |
| ATOM | 113 | N   | PHE | A | 33 | 3.409  | 39.806 | -1.884 | 1.00 | 32.01 |
| ATOM | 114 | CA  | PHE | A | 33 | 4.435  | 39.728 | -0.852 | 1.00 | 31.66 |
| ATOM | 115 | CB  | PHE | A | 33 | 5.168  | 38.384 | -0.942 | 1.00 | 32.90 |
| ATOM | 116 | CG  | PHE | A | 33 | 6.024  | 38.057 | 0.254  | 1.00 | 30.75 |
| ATOM | 117 | CD1 | PHE | A | 33 | 5.708  | 38.529 | 1.524  | 1.00 | 34.33 |
| ATOM | 118 | CE1 | PHE | A | 33 | 6.507  | 38.213 | 2.616  | 1.00 | 34.24 |
| ATOM | 119 | CZ  | PHE | A | 33 | 7.643  | 37.424 | 2.450  | 1.00 | 35.46 |
| ATOM | 120 | CE2 | PHE | A | 33 | 7.961  | 36.943 | 1.186  | 1.00 | 32.02 |
| ATOM | 121 | CD2 | PHE | A | 33 | 7.145  | 37.255 | 0.106  | 1.00 | 27.29 |
| ATOM | 122 | C   | PHE | A | 33 | 5.395  | 40.917 | -0.953 | 1.00 | 31.91 |
| ATOM | 123 | O   | PHE | A | 33 | 5.757  | 41.484 | 0.077  | 1.00 | 30.81 |
| ATOM | 124 | N   | MET | A | 34 | 5.784  | 41.309 | -2.170 | 1.00 | 31.13 |
| ATOM | 125 | CA  | MET | A | 34 | 6.599  | 42.512 | -2.328 | 1.00 | 34.10 |
| ATOM | 126 | CB  | MET | A | 34 | 6.951  | 42.790 | -3.797 | 1.00 | 33.71 |
| ATOM | 127 | CG  | MET | A | 34 | 7.918  | 41.787 | -4.410 | 1.00 | 36.64 |
| ATOM | 128 | SD  | MET | A | 34 | 9.456  | 41.519 | -3.504 | 1.00 | 45.35 |
| ATOM | 129 | CE  | MET | A | 34 | 10.582 | 40.969 | -4.820 | 1.00 | 46.02 |
| ATOM | 130 | C   | MET | A | 34 | 5.903  | 43.709 | -1.674 | 1.00 | 33.09 |
| ATOM | 131 | O   | MET | A | 34 | 6.504  | 44.406 | -0.866 | 1.00 | 34.24 |
| ATOM | 132 | N   | LYS | A | 35 | 4.629  | 43.919 | -1.996 | 1.00 | 35.14 |
| ATOM | 133 | CA  | LYS | A | 35 | 3.835  | 44.999 | -1.411 | 1.00 | 35.12 |
| ATOM | 134 | CB  | LYS | A | 35 | 2.416  | 44.986 | -1.990 | 1.00 | 36.58 |
| ATOM | 135 | CG  | LYS | A | 35 | 2.372  | 45.164 | -3.500 | 1.00 | 39.86 |
| ATOM | 136 | CD  | LYS | A | 35 | 1.013  | 45.684 | -3.944 | 1.00 | 44.78 |
| ATOM | 137 | CE  | LYS | A | 35 | 1.181  | 46.751 | -5.007 | 1.00 | 46.40 |
| ATOM | 138 | NZ  | LYS | A | 35 | 1.355  | 46.127 | -6.352 | 1.00 | 48.36 |
| ATOM | 139 | C   | LYS | A | 35 | 3.808  | 44.960 | 0.122  | 1.00 | 35.83 |
| ATOM | 140 | O   | LYS | A | 35 | 4.075  | 45.958 | 0.793  | 1.00 | 34.45 |
| ATOM | 141 | N   | LEU | A | 36 | 3.505  | 43.799 | 0.695  | 1.00 | 34.49 |
| ATOM | 142 | CA  | LEU | A | 36 | 3.546  | 43.658 | 2.144  | 1.00 | 33.34 |
| ATOM | 143 | CB  | LEU | A | 36 | 3.238  | 42.218 | 2.534  | 1.00 | 33.70 |
| ATOM | 144 | CG  | LEU | A | 36 | 1.800  | 41.748 | 2.349  | 1.00 | 34.08 |
| ATOM | 145 | CD1 | LEU | A | 36 | 1.759  | 40.272 | 2.714  | 1.00 | 39.25 |
| ATOM | 146 | CD2 | LEU | A | 36 | 0.827  | 42.549 | 3.202  | 1.00 | 35.36 |
| ATOM | 147 | C   | LEU | A | 36 | 4.908  | 44.006 | 2.720  | 1.00 | 34.23 |
| ATOM | 148 | O   | LEU | A | 36 | 5.017  | 44.469 | 3.855  | 1.00 | 32.77 |
| ATOM | 149 | N   | GLN | A | 37 | 5.952  | 43.758 | 1.934  | 1.00 | 36.11 |
| ATOM | 150 | CA  | GLN | A | 37 | 7.315  | 43.871 | 2.434  | 1.00 | 38.15 |
| ATOM | 151 | CB  | GLN | A | 37 | 8.226  | 42.852 | 1.746  | 1.00 | 39.69 |
| ATOM | 152 | CG  | GLN | A | 37 | 8.393  | 41.537 | 2.507  | 1.00 | 41.08 |
| ATOM | 153 | CD  | GLN | A | 37 | 9.248  | 40.543 | 1.750  | 1.00 | 42.50 |
| ATOM | 154 | OE1 | GLN | A | 37 | 10.228 | 40.029 | 2.281  | 1.00 | 46.33 |
| ATOM | 155 | NE2 | GLN | A | 37 | 8.882  | 40.274 | 0.505  | 1.00 | 46.39 |

**FIGURE 255**

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|      |     |     |     |   |    |        |        |       |      |       |
|------|-----|-----|-----|---|----|--------|--------|-------|------|-------|
| ATOM | 156 | C   | GLN | A | 37 | 7.888  | 45.280 | 2.283 | 1.00 | 39.26 |
| ATOM | 157 | O   | GLN | A | 37 | 8.913  | 45.600 | 2.881 | 1.00 | 38.73 |
| ATOM | 158 | N   | ALA | A | 38 | 7.219  | 46.099 | 1.481 | 1.00 | 39.85 |
| ATOM | 159 | CA  | ALA | A | 38 | 7.634  | 47.480 | 1.237 | 1.00 | 41.68 |
| ATOM | 160 | CB  | ALA | A | 38 | 6.717  | 48.129 | 0.200 | 1.00 | 40.33 |
| ATOM | 161 | C   | ALA | A | 38 | 7.638  | 48.288 | 2.538 | 1.00 | 42.41 |
| ATOM | 162 | O   | ALA | A | 38 | 7.000  | 47.898 | 3.515 | 1.00 | 42.66 |
| ATOM | 163 | N   | ASP | A | 39 | 8.358  | 49.408 | 2.545 | 1.00 | 43.16 |
| ATOM | 164 | CA  | ASP | A | 39 | 8.490  | 50.253 | 3.731 | 1.00 | 43.58 |
| ATOM | 165 | CB  | ASP | A | 39 | 7.222  | 51.066 | 3.995 | 1.00 | 43.94 |
| ATOM | 166 | CG  | ASP | A | 39 | 6.539  | 51.521 | 2.733 | 1.00 | 46.50 |
| ATOM | 167 | OD1 | ASP | A | 39 | 5.474  | 52.165 | 2.853 | 1.00 | 53.13 |
| ATOM | 168 | OD2 | ASP | A | 39 | 6.982  | 51.279 | 1.592 | 1.00 | 51.25 |
| ATOM | 169 | C   | ASP | A | 39 | 8.782  | 49.487 | 5.011 | 1.00 | 43.69 |
| ATOM | 170 | O   | ASP | A | 39 | 8.062  | 49.653 | 5.991 | 1.00 | 44.78 |
| ATOM | 171 | N   | SER | A | 40 | 9.823  | 48.663 | 5.025 | 1.00 | 44.51 |
| ATOM | 172 | CA  | SER | A | 40 | 10.177 | 47.964 | 6.256 | 1.00 | 44.47 |
| ATOM | 173 | CB  | SER | A | 40 | 10.697 | 48.954 | 7.308 | 1.00 | 45.60 |
| ATOM | 174 | OG  | SER | A | 40 | 11.858 | 49.640 | 6.852 | 1.00 | 45.70 |
| ATOM | 175 | C   | SER | A | 40 | 8.934  | 47.224 | 6.770 | 1.00 | 44.23 |
| ATOM | 176 | O   | SER | A | 40 | 8.450  | 47.477 | 7.879 | 1.00 | 43.64 |
| ATOM | 177 | N   | ASN | A | 41 | 8.410  | 46.338 | 5.927 | 1.00 | 42.57 |
| ATOM | 178 | CA  | ASN | A | 41 | 7.313  | 45.448 | 6.293 | 1.00 | 41.50 |
| ATOM | 179 | CB  | ASN | A | 41 | 7.802  | 44.364 | 7.264 | 1.00 | 42.19 |
| ATOM | 180 | CG  | ASN | A | 41 | 8.525  | 43.225 | 6.559 | 1.00 | 43.25 |
| ATOM | 181 | OD1 | ASN | A | 41 | 8.753  | 43.268 | 5.350 | 1.00 | 47.07 |
| ATOM | 182 | ND2 | ASN | A | 41 | 8.897  | 42.200 | 7.317 | 1.00 | 44.15 |
| ATOM | 183 | C   | ASN | A | 41 | 6.051  | 46.146 | 6.805 | 1.00 | 40.97 |
| ATOM | 184 | O   | ASN | A | 41 | 5.262  | 45.570 | 7.559 | 1.00 | 40.09 |
| ATOM | 185 | N   | TYR | A | 42 | 5.842  | 47.383 | 6.370 | 1.00 | 39.82 |
| ATOM | 186 | CA  | TYR | A | 42 | 4.723  | 48.184 | 6.859 | 1.00 | 40.35 |
| ATOM | 187 | CB  | TYR | A | 42 | 4.655  | 49.528 | 6.125 | 1.00 | 41.74 |
| ATOM | 188 | CG  | TYR | A | 42 | 3.461  | 50.359 | 6.527 | 1.00 | 45.15 |
| ATOM | 189 | CD1 | TYR | A | 42 | 3.431  | 51.021 | 7.753 | 1.00 | 48.34 |
| ATOM | 190 | CE1 | TYR | A | 42 | 2.333  | 51.778 | 8.137 | 1.00 | 51.74 |
| ATOM | 191 | CZ  | TYR | A | 42 | 1.246  | 51.877 | 7.287 | 1.00 | 54.21 |
| ATOM | 192 | OH  | TYR | A | 42 | 0.154  | 52.632 | 7.659 | 1.00 | 55.81 |
| ATOM | 193 | CE2 | TYR | A | 42 | 1.250  | 51.227 | 6.065 | 1.00 | 52.92 |
| ATOM | 194 | CD2 | TYR | A | 42 | 2.358  | 50.472 | 5.690 | 1.00 | 49.40 |
| ATOM | 195 | C   | TYR | A | 42 | 3.369  | 47.472 | 6.809 | 1.00 | 38.41 |
| ATOM | 196 | O   | TYR | A | 42 | 2.685  | 47.355 | 7.826 | 1.00 | 37.47 |
| ATOM | 197 | N   | LEU | A | 43 | 2.985  | 46.978 | 5.635 | 1.00 | 37.22 |
| ATOM | 198 | CA  | LEU | A | 43 | 1.667  | 46.380 | 5.480 | 1.00 | 34.65 |
| ATOM | 199 | CB  | LEU | A | 43 | 1.205  | 46.392 | 4.021 | 1.00 | 36.77 |
| ATOM | 200 | CG  | LEU | A | 43 | 0.731  | 47.739 | 3.455 | 1.00 | 34.94 |
| ATOM | 201 | CD1 | LEU | A | 43 | 0.530  | 47.603 | 1.962 | 1.00 | 38.85 |
| ATOM | 202 | CD2 | LEU | A | 43 | -0.567 | 48.164 | 4.139 | 1.00 | 37.34 |
| ATOM | 203 | C   | LEU | A | 43 | 1.660  | 44.953 | 6.016 | 1.00 | 34.58 |
| ATOM | 204 | O   | LEU | A | 43 | 0.613  | 44.459 | 6.441 | 1.00 | 33.18 |
| ATOM | 205 | N   | LEU | A | 44 | 2.812  | 44.290 | 5.972 | 1.00 | 32.70 |
| ATOM | 206 | CA  | LEU | A | 44 | 2.917  | 42.976 | 6.606 | 1.00 | 32.37 |
| ATOM | 207 | CB  | LEU | A | 44 | 4.316  | 42.376 | 6.458 | 1.00 | 32.08 |

**FIGURE 256**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 208 | CG  | LEU | A | 44 | 4.293  | 40.922 | 6.948  | 1.00 | 30.67 |
| ATOM | 209 | CD1 | LEU | A | 44 | 4.884  | 39.953 | 5.934  | 1.00 | 35.30 |
| ATOM | 210 | CD2 | LEU | A | 44 | 4.877  | 40.746 | 8.342  | 1.00 | 30.73 |
| ATOM | 211 | C   | LEU | A | 44 | 2.574  | 43.078 | 8.092  | 1.00 | 33.04 |
| ATOM | 212 | O   | LEU | A | 44 | 1.743  | 42.326 | 8.603  | 1.00 | 31.84 |
| ATOM | 213 | N   | SER | A | 45 | 3.248  | 43.992 | 8.784  | 1.00 | 32.72 |
| ATOM | 214 | CA  | SER | A | 45 | 3.023  | 44.200 | 10.211 | 1.00 | 32.14 |
| ATOM | 215 | CB  | SER | A | 45 | 3.937  | 45.297 | 10.761 | 1.00 | 32.86 |
| ATOM | 216 | OG  | SER | A | 45 | 5.298  | 44.946 | 10.616 | 1.00 | 33.52 |
| ATOM | 217 | C   | SER | A | 45 | 1.579  | 44.543 | 10.543 | 1.00 | 31.96 |
| ATOM | 218 | O   | SER | A | 45 | 1.063  | 44.085 | 11.562 | 1.00 | 31.93 |
| ATOM | 219 | N   | LYS | A | 46 | 0.937  | 45.378 | 9.730  | 1.00 | 31.67 |
| ATOM | 220 | CA  | LYS | A | 46 | -0.452 | 45.743 | 9.983  | 1.00 | 32.52 |
| ATOM | 221 | CB  | LYS | A | 46 | -0.907 | 46.880 | 9.058  | 1.00 | 33.10 |
| ATOM | 222 | CG  | LYS | A | 46 | -0.320 | 48.247 | 9.408  | 1.00 | 37.46 |
| ATOM | 223 | CD  | LYS | A | 46 | -1.206 | 49.024 | 10.362 | 1.00 | 43.28 |
| ATOM | 224 | CE  | LYS | A | 46 | -0.660 | 48.938 | 11.785 | 1.00 | 46.45 |
| ATOM | 225 | NZ  | LYS | A | 46 | -1.645 | 48.309 | 12.714 | 1.00 | 43.98 |
| ATOM | 226 | C   | LYS | A | 46 | -1.361 | 44.534 | 9.819  | 1.00 | 31.81 |
| ATOM | 227 | O   | LYS | A | 46 | -2.279 | 44.313 | 10.608 | 1.00 | 33.52 |
| ATOM | 228 | N   | GLU | A | 47 | -1.108 | 43.735 | 8.788  | 1.00 | 30.77 |
| ATOM | 229 | CA  | GLU | A | 47 | -1.921 | 42.546 | 8.607  | 1.00 | 29.42 |
| ATOM | 230 | CB  | GLU | A | 47 | -1.527 | 41.852 | 7.317  | 1.00 | 29.31 |
| ATOM | 231 | CG  | GLU | A | 47 | -2.261 | 40.540 | 7.157  | 1.00 | 30.91 |
| ATOM | 232 | CD  | GLU | A | 47 | -2.032 | 39.991 | 5.770  | 1.00 | 33.04 |
| ATOM | 233 | OE1 | GLU | A | 47 | -2.462 | 40.656 | 4.790  | 1.00 | 31.27 |
| ATOM | 234 | OE2 | GLU | A | 47 | -1.387 | 38.923 | 5.697  | 1.00 | 30.22 |
| ATOM | 235 | C   | GLU | A | 47 | -1.745 | 41.573 | 9.764  | 1.00 | 27.29 |
| ATOM | 236 | O   | GLU | A | 47 | -2.729 | 41.065 | 10.317 | 1.00 | 28.88 |
| ATOM | 237 | N   | TYR | A | 48 | -0.488 | 41.316 | 10.110 | 1.00 | 27.52 |
| ATOM | 238 | CA  | TYR | A | 48 | -0.170 | 40.444 | 11.234 | 1.00 | 28.53 |
| ATOM | 239 | CB  | TYR | A | 48 | 1.337  | 40.327 | 11.426 | 1.00 | 26.41 |
| ATOM | 240 | CG  | TYR | A | 48 | 1.697  | 39.418 | 12.574 | 1.00 | 30.88 |
| ATOM | 241 | CD1 | TYR | A | 48 | 1.508  | 38.039 | 12.489 | 1.00 | 27.50 |
| ATOM | 242 | CE1 | TYR | A | 48 | 1.854  | 37.212 | 13.547 | 1.00 | 26.46 |
| ATOM | 243 | CZ  | TYR | A | 48 | 2.341  | 37.759 | 14.713 | 1.00 | 31.48 |
| ATOM | 244 | OH  | TYR | A | 48 | 2.683  | 36.975 | 15.797 | 1.00 | 33.16 |
| ATOM | 245 | CE2 | TYR | A | 48 | 2.539  | 39.118 | 14.814 | 1.00 | 33.37 |
| ATOM | 246 | CD2 | TYR | A | 48 | 2.198  | 39.937 | 13.760 | 1.00 | 31.15 |
| ATOM | 247 | C   | TYR | A | 48 | -0.807 | 40.876 | 12.555 | 1.00 | 30.00 |
| ATOM | 248 | O   | TYR | A | 48 | -1.212 | 40.047 | 13.374 | 1.00 | 29.71 |
| ATOM | 249 | N   | GLU | A | 49 | -0.867 | 42.179 | 12.800 | 1.00 | 29.94 |
| ATOM | 250 | CA  | GLU | A | 49 | -1.423 | 42.607 | 14.082 | 1.00 | 29.29 |
| ATOM | 251 | CB  | GLU | A | 49 | -0.863 | 43.970 | 14.510 | 1.00 | 31.83 |
| ATOM | 252 | CG  | GLU | A | 49 | 0.648  | 43.941 | 14.759 | 1.00 | 34.43 |
| ATOM | 253 | CD  | GLU | A | 49 | 1.103  | 43.090 | 15.942 | 1.00 | 41.82 |
| ATOM | 254 | OE1 | GLU | A | 49 | 2.329  | 42.964 | 16.146 | 1.00 | 45.44 |
| ATOM | 255 | OE2 | GLU | A | 49 | 0.267  | 42.555 | 16.705 | 1.00 | 49.14 |
| ATOM | 256 | C   | GLU | A | 49 | -2.948 | 42.494 | 14.156 | 1.00 | 28.43 |
| ATOM | 257 | O   | GLU | A | 49 | -3.519 | 42.445 | 15.243 | 1.00 | 28.47 |
| ATOM | 258 | N   | GLU | A | 50 | -3.597 | 42.362 | 13.002 | 1.00 | 26.77 |
| ATOM | 259 | CA  | GLU | A | 50 | -5.026 | 42.129 | 12.939 | 1.00 | 28.42 |

**FIGURE 257**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 260 | CB  | GLU | A | 50 | -5.501 | 42.167 | 11.493 | 1.00 | 29.72 |
| ATOM | 261 | CG  | GLU | A | 50 | -5.695 | 43.555 | 10.902 | 1.00 | 37.08 |
| ATOM | 262 | CD  | GLU | A | 50 | -6.521 | 43.494 | 9.635  | 1.00 | 48.22 |
| ATOM | 263 | OE1 | GLU | A | 50 | -7.094 | 44.536 | 9.235  | 1.00 | 53.56 |
| ATOM | 264 | OE2 | GLU | A | 50 | -6.588 | 42.394 | 9.038  | 1.00 | 51.31 |
| ATOM | 265 | C   | GLU | A | 50 | -5.369 | 40.744 | 13.487 | 1.00 | 26.59 |
| ATOM | 266 | O   | GLU | A | 50 | -6.498 | 40.514 | 13.903 | 1.00 | 28.10 |
| ATOM | 267 | N   | LEU | A | 51 | -4.385 | 39.855 | 13.481 | 1.00 | 26.25 |
| ATOM | 268 | CA  | LEU | A | 51 | -4.561 | 38.486 | 13.994 | 1.00 | 23.60 |
| ATOM | 269 | CB  | LEU | A | 51 | -3.585 | 37.538 | 13.284 | 1.00 | 22.99 |
| ATOM | 270 | CG  | LEU | A | 51 | -3.829 | 37.234 | 11.798 | 1.00 | 22.34 |
| ATOM | 271 | CD1 | LEU | A | 51 | -2.549 | 36.611 | 11.228 | 1.00 | 18.21 |
| ATOM | 272 | CD2 | LEU | A | 51 | -5.087 | 36.385 | 11.612 | 1.00 | 24.13 |
| ATOM | 273 | C   | LEU | A | 51 | -4.370 | 38.363 | 15.509 | 1.00 | 24.96 |
| ATOM | 274 | O   | LEU | A | 51 | -4.677 | 37.326 | 16.111 | 1.00 | 22.08 |
| ATOM | 275 | N   | LYS | A | 52 | -3.855 | 39.417 | 16.144 | 1.00 | 26.20 |
| ATOM | 276 | CA  | LYS | A | 52 | -3.365 | 39.323 | 17.514 | 1.00 | 26.71 |
| ATOM | 277 | CB  | LYS | A | 52 | -2.860 | 40.693 | 17.980 | 1.00 | 26.43 |
| ATOM | 278 | CG  | LYS | A | 52 | -2.737 | 40.861 | 19.471 | 1.00 | 33.28 |
| ATOM | 279 | CD  | LYS | A | 52 | -2.346 | 42.297 | 19.849 | 1.00 | 36.15 |
| ATOM | 280 | CE  | LYS | A | 52 | -2.370 | 42.442 | 21.371 | 1.00 | 39.71 |
| ATOM | 281 | NZ  | LYS | A | 52 | -3.746 | 42.725 | 21.891 | 1.00 | 41.67 |
| ATOM | 282 | C   | LYS | A | 52 | -4.401 | 38.751 | 18.487 | 1.00 | 25.95 |
| ATOM | 283 | O   | LYS | A | 52 | -4.071 | 37.922 | 19.335 | 1.00 | 28.87 |
| ATOM | 284 | N   | ASP | A | 53 | -5.647 | 39.193 | 18.369 | 1.00 | 25.82 |
| ATOM | 285 | CA  | ASP | A | 53 | -6.665 | 38.840 | 19.352 | 1.00 | 27.69 |
| ATOM | 286 | CB  | ASP | A | 53 | -7.547 | 40.052 | 19.677 | 1.00 | 29.82 |
| ATOM | 287 | CG  | ASP | A | 53 | -6.811 | 41.109 | 20.492 | 1.00 | 35.24 |
| ATOM | 288 | OD1 | ASP | A | 53 | -7.138 | 42.300 | 20.303 | 1.00 | 41.07 |
| ATOM | 289 | OD2 | ASP | A | 53 | -5.893 | 40.851 | 21.306 | 1.00 | 38.05 |
| ATOM | 290 | C   | ASP | A | 53 | -7.569 | 37.670 | 18.980 | 1.00 | 25.40 |
| ATOM | 291 | O   | ASP | A | 53 | -8.525 | 37.364 | 19.698 | 1.00 | 26.92 |
| ATOM | 292 | N   | VAL | A | 54 | -7.297 | 37.026 | 17.853 | 1.00 | 21.25 |
| ATOM | 293 | CA  | VAL | A | 54 | -8.181 | 35.958 | 17.403 | 1.00 | 20.37 |
| ATOM | 294 | CB  | VAL | A | 54 | -7.674 | 35.400 | 16.059 | 1.00 | 20.28 |
| ATOM | 295 | CG1 | VAL | A | 54 | -8.452 | 34.176 | 15.627 | 1.00 | 20.13 |
| ATOM | 296 | CG2 | VAL | A | 54 | -7.640 | 36.526 | 14.988 | 1.00 | 20.70 |
| ATOM | 297 | C   | VAL | A | 54 | -8.155 | 34.888 | 18.496 | 1.00 | 21.34 |
| ATOM | 298 | O   | VAL | A | 54 | -7.068 | 34.539 | 18.969 | 1.00 | 21.56 |
| ATOM | 299 | N   | GLY | A | 55 | -9.345 | 34.408 | 18.857 | 1.00 | 19.73 |
| ATOM | 300 | CA  | GLY | A | 55 | -9.501 | 33.351 | 19.830 | 1.00 | 21.36 |
| ATOM | 301 | C   | GLY | A | 55 | -9.516 | 33.779 | 21.284 | 1.00 | 25.60 |
| ATOM | 302 | O   | GLY | A | 55 | -9.779 | 32.934 | 22.137 | 1.00 | 25.18 |
| ATOM | 303 | N   | ARG | A | 56 | -9.243 | 35.041 | 21.597 | 1.00 | 28.66 |
| ATOM | 304 | CA  | ARG | A | 56 | -8.825 | 35.351 | 22.967 | 1.00 | 33.28 |
| ATOM | 305 | CB  | ARG | A | 56 | -7.723 | 36.420 | 23.019 | 1.00 | 34.38 |
| ATOM | 306 | CG  | ARG | A | 56 | -6.566 | 36.172 | 22.048 | 1.00 | 38.44 |
| ATOM | 307 | CD  | ARG | A | 56 | -5.400 | 35.366 | 22.594 | 1.00 | 41.11 |
| ATOM | 308 | NE  | ARG | A | 56 | -4.139 | 35.991 | 22.211 | 1.00 | 47.68 |
| ATOM | 309 | CZ  | ARG | A | 56 | -3.441 | 36.808 | 22.989 | 1.00 | 51.01 |
| ATOM | 310 | NH1 | ARG | A | 56 | -3.880 | 37.097 | 24.206 | 1.00 | 50.37 |
| ATOM | 311 | NH2 | ARG | A | 56 | -2.308 | 37.346 | 22.551 | 1.00 | 48.68 |

**FIGURE 258**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 312 | C   | ARG | A | 56 | -10.003 | 35.704 | 23.870 | 1.00 | 34.09 |
| ATOM | 313 | O   | ARG | A | 56 | -9.826  | 36.081 | 25.030 | 1.00 | 37.38 |
| ATOM | 314 | N   | ASN | A | 57 | -11.198 | 35.540 | 23.319 | 1.00 | 34.85 |
| ATOM | 315 | CA  | ASN | A | 57 | -12.448 | 35.609 | 24.046 | 1.00 | 34.43 |
| ATOM | 316 | CB  | ASN | A | 57 | -13.561 | 35.897 | 23.039 | 1.00 | 35.95 |
| ATOM | 317 | CG  | ASN | A | 57 | -13.661 | 34.836 | 21.944 | 1.00 | 40.08 |
| ATOM | 318 | OD1 | ASN | A | 57 | -12.748 | 34.655 | 21.124 | 1.00 | 42.89 |
| ATOM | 319 | ND2 | ASN | A | 57 | -14.799 | 34.144 | 21.912 | 1.00 | 40.39 |
| ATOM | 320 | C   | ASN | A | 57 | -12.760 | 34.309 | 24.799 | 1.00 | 31.67 |
| ATOM | 321 | O   | ASN | A | 57 | -13.767 | 34.232 | 25.487 | 1.00 | 33.78 |
| ATOM | 322 | N   | GLN | A | 58 | -11.920 | 33.286 | 24.653 | 1.00 | 27.75 |
| ATOM | 323 | CA  | GLN | A | 58 | -12.243 | 31.931 | 25.119 | 1.00 | 24.28 |
| ATOM | 324 | CB  | GLN | A | 58 | -11.843 | 30.903 | 24.058 | 1.00 | 23.90 |
| ATOM | 325 | CG  | GLN | A | 58 | -12.595 | 31.051 | 22.743 | 1.00 | 25.65 |
| ATOM | 326 | CD  | GLN | A | 58 | -12.102 | 30.074 | 21.714 | 1.00 | 26.89 |
| ATOM | 327 | OE1 | GLN | A | 58 | -10.971 | 30.202 | 21.238 | 1.00 | 28.76 |
| ATOM | 328 | NE2 | GLN | A | 58 | -12.933 | 29.084 | 21.381 | 1.00 | 28.16 |
| ATOM | 329 | C   | GLN | A | 58 | -11.584 | 31.583 | 26.458 | 1.00 | 23.11 |
| ATOM | 330 | O   | GLN | A | 58 | -10.450 | 32.001 | 26.725 | 1.00 | 21.96 |
| ATOM | 331 | N   | SER | A | 59 | -12.285 | 30.801 | 27.284 | 1.00 | 21.91 |
| ATOM | 332 | CA  | SER | A | 59 | -11.880 | 30.520 | 28.667 | 1.00 | 21.56 |
| ATOM | 333 | CB  | SER | A | 59 | -13.120 | 30.331 | 29.548 | 1.00 | 25.89 |
| ATOM | 334 | OG  | SER | A | 59 | -13.853 | 29.160 | 29.159 | 1.00 | 30.06 |
| ATOM | 335 | C   | SER | A | 59 | -10.966 | 29.293 | 28.744 | 1.00 | 20.75 |
| ATOM | 336 | O   | SER | A | 59 | -11.067 | 28.413 | 27.879 | 1.00 | 21.59 |
| ATOM | 337 | N   | CYS | A | 60 | -10.045 | 29.281 | 29.717 | 1.00 | 17.44 |
| ATOM | 338 | CA  | CYS | A | 60 | -9.241  | 28.110 | 30.066 | 1.00 | 16.53 |
| ATOM | 339 | CB  | CYS | A | 60 | -7.727  | 28.401 | 29.837 | 1.00 | 16.03 |
| ATOM | 340 | SG  | CYS | A | 60 | -7.335  | 28.999 | 28.191 | 1.00 | 20.55 |
| ATOM | 341 | C   | CYS | A | 60 | -9.464  | 27.783 | 31.540 | 1.00 | 15.89 |
| ATOM | 342 | O   | CYS | A | 60 | -8.518  | 27.605 | 32.301 | 1.00 | 16.90 |
| ATOM | 343 | N   | ASP | A | 61 | -10.724 | 27.666 | 31.948 | 1.00 | 16.95 |
| ATOM | 344 | CA  | ASP | A | 61 | -11.008 | 27.467 | 33.364 | 1.00 | 18.02 |
| ATOM | 345 | CB  | ASP | A | 61 | -12.496 | 27.660 | 33.610 | 1.00 | 19.47 |
| ATOM | 346 | CG  | ASP | A | 61 | -12.954 | 29.082 | 33.379 | 1.00 | 24.64 |
| ATOM | 347 | OD1 | ASP | A | 61 | -12.160 | 30.049 | 33.365 | 1.00 | 20.11 |
| ATOM | 348 | OD2 | ASP | A | 61 | -14.155 | 29.306 | 33.171 | 1.00 | 24.81 |
| ATOM | 349 | C   | ASP | A | 61 | -10.574 | 26.102 | 33.887 | 1.00 | 20.07 |
| ATOM | 350 | O   | ASP | A | 61 | -10.102 | 25.997 | 35.017 | 1.00 | 21.40 |
| ATOM | 351 | N   | ILE | A | 62 | -10.679 | 25.062 | 33.064 | 1.00 | 17.97 |
| ATOM | 352 | CA  | ILE | A | 62 | -10.298 | 23.747 | 33.574 | 1.00 | 16.98 |
| ATOM | 353 | CB  | ILE | A | 62 | -10.723 | 22.652 | 32.564 | 1.00 | 14.99 |
| ATOM | 354 | CG1 | ILE | A | 62 | -12.247 | 22.609 | 32.414 | 1.00 | 19.52 |
| ATOM | 355 | CD1 | ILE | A | 62 | -12.918 | 22.254 | 33.696 | 1.00 | 24.86 |
| ATOM | 356 | CG2 | ILE | A | 62 | -10.213 | 21.266 | 32.987 | 1.00 | 18.74 |
| ATOM | 357 | C   | ILE | A | 62 | -8.779  | 23.712 | 33.804 | 1.00 | 17.57 |
| ATOM | 358 | O   | ILE | A | 62 | -8.295  | 23.179 | 34.802 | 1.00 | 18.69 |
| ATOM | 359 | N   | ALA | A | 63 | -8.036  | 24.245 | 32.841 | 1.00 | 16.86 |
| ATOM | 360 | CA  | ALA | A | 63 | -6.570  | 24.285 | 32.923 | 1.00 | 18.52 |
| ATOM | 361 | CB  | ALA | A | 63 | -5.999  | 24.905 | 31.623 | 1.00 | 18.66 |
| ATOM | 362 | C   | ALA | A | 63 | -6.075  | 25.067 | 34.155 | 1.00 | 19.62 |
| ATOM | 363 | O   | ALA | A | 63 | -4.972  | 24.842 | 34.653 | 1.00 | 20.46 |

**FIGURE 259**

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Three Dimensional Coordinates of HPTPbeta

|      |     |         |      |    |    |         |        |        |      |       |
|------|-----|---------|------|----|----|---------|--------|--------|------|-------|
| ATOM | 364 | N       | LEU  | A  | 64 | -6.919  | 25.972 | 34.632 | 1.00 | 20.64 |
| ATOM | 365 | CA      | LEU  | A  | 64 | -6.605  | 26.811 | 35.779 | 1.00 | 21.59 |
| ATOM | 366 | CB      | LEU  | A  | 64 | -7.316  | 28.157 | 35.640 | 1.00 | 21.74 |
| ATOM | 367 | CG      | LEU  | A  | 64 | -6.603  | 29.150 | 34.735 | 1.00 | 22.91 |
| ATOM | 368 | CD1     | LEU  | A  | 64 | -7.504  | 30.360 | 34.530 | 1.00 | 26.23 |
| ATOM | 369 | CD2     | LEU  | A  | 64 | -5.274  | 29.607 | 35.346 | 1.00 | 20.97 |
| ATOM | 370 | C       | LEU  | A  | 64 | -6.988  | 26.205 | 37.128 | 1.00 | 23.83 |
| ATOM | 371 | O       | LEU  | A  | 64 | -6.666  | 26.792 | 38.168 | 1.00 | 24.37 |
| ATOM | 372 | N       | LEU  | A  | 65 | -7.690  | 25.071 | 37.144 | 1.00 | 23.26 |
| ATOM | 373 | CA      | LEU  | A  | 65 | -8.009  | 24.427 | 38.418 | 1.00 | 25.30 |
| ATOM | 374 | CB      | LEU  | A  | 65 | -8.892  | 23.199 | 38.218 | 1.00 | 23.61 |
| ATOM | 375 | CG      | LEU  | A  | 65 | -10.281 | 23.423 | 37.623 | 1.00 | 25.74 |
| ATOM | 376 | CD1     | LEU  | A  | 65 | -10.875 | 22.077 | 37.228 | 1.00 | 27.81 |
| ATOM | 377 | CD2     | LEU  | A  | 65 | -11.154 | 24.183 | 38.616 | 1.00 | 27.81 |
| ATOM | 378 | C       | LEU  | A  | 65 | -6.739  | 24.069 | 39.184 | 1.00 | 25.22 |
| ATOM | 379 | O       | LEU  | A  | 65 | -5.741  | 23.654 | 38.606 | 1.00 | 23.18 |
| ATOM | 380 | N       | PRO  | A  | 66 | -6.716  | 24.280 | 40.498 | 1.00 | 26.80 |
| ATOM | 381 | CA      | PRO  | A  | 66 | -5.463  | 24.105 | 41.234 | 1.00 | 26.96 |
| ATOM | 382 | CB      | PRO  | A  | 66 | -5.830  | 24.483 | 42.678 | 1.00 | 28.00 |
| ATOM | 383 | CG      | PRO  | A  | 66 | -7.289  | 24.642 | 42.717 | 1.00 | 27.81 |
| ATOM | 384 | CD      | PRO  | A  | 66 | -7.827  | 24.762 | 41.333 | 1.00 | 29.27 |
| ATOM | 385 | C       | PRO  | A  | 66 | -4.917  | 22.683 | 41.121 | 1.00 | 27.13 |
| ATOM | 386 | O       | PRO  | A  | 66 | -3.697  | 22.517 | 41.088 | 1.00 | 25.29 |
| ATOM | 387 | N       | GLU  | A  | 67 | -5.819  | 21.707 | 41.019 | 1.00 | 27.81 |
| ATOM | 388 | CA      | GLU  | A  | 67 | -5.504  | 20.294 | 40.825 | 1.00 | 28.93 |
| ATOM | 389 | CB      | GLU  | A  | 67 | -6.818  | 19.510 | 40.733 | 1.00 | 30.51 |
| ATOM | 390 | CG      | AGLU | A  | 67 | -6.790  | 18.040 | 41.147 | 0.50 | 32.82 |
| ATOM | 391 | CG      | BGLU | A  | 67 | -7.575  | 19.363 | 42.052 | 0.50 | 29.81 |
| ATOM | 392 | CD      | AGLU | A  | 67 | -5.497  | 17.580 | 41.804 | 0.50 | 34.06 |
| ATOM | 393 | CD      | BGLU | A  | 67 | -8.575  | 20.471 | 42.362 | 0.50 | 32.38 |
| ATOM | 394 | OE1AGLU | A    | 67 | 67 | -5.465  | 17.473 | 43.049 | 0.50 | 33.59 |
| ATOM | 395 | OE1BGLU | A    | 67 | 67 | -8.580  | 21.554 | 41.729 | 0.50 | 28.29 |
| ATOM | 396 | OE2AGLU | A    | 67 | 67 | -4.523  | 17.281 | 41.077 | 0.50 | 37.14 |
| ATOM | 397 | OE2BGLU | A    | 67 | 67 | -9.376  | 20.260 | 43.298 | 0.50 | 33.73 |
| ATOM | 398 | C       | GLU  | A  | 67 | -4.681  | 20.052 | 39.557 | 1.00 | 28.81 |
| ATOM | 399 | O       | GLU  | A  | 67 | -3.896  | 19.100 | 39.474 | 1.00 | 28.70 |
| ATOM | 400 | N       | ASN  | A  | 68 | -4.841  | 20.938 | 38.577 | 1.00 | 27.24 |
| ATOM | 401 | CA      | ASN  | A  | 68 | -4.105  | 20.833 | 37.324 | 1.00 | 26.55 |
| ATOM | 402 | CB      | ASN  | A  | 68 | -5.043  | 21.171 | 36.157 | 1.00 | 23.97 |
| ATOM | 403 | CG      | ASN  | A  | 68 | -6.154  | 20.139 | 35.977 | 1.00 | 25.76 |
| ATOM | 404 | OD1     | ASN  | A  | 68 | -5.976  | 18.936 | 36.227 | 1.00 | 21.62 |
| ATOM | 405 | ND2     | ASN  | A  | 68 | -7.312  | 20.596 | 35.510 | 1.00 | 21.09 |
| ATOM | 406 | C       | ASN  | A  | 68 | -2.780  | 21.602 | 37.228 | 1.00 | 25.64 |
| ATOM | 407 | O       | ASN  | A  | 68 | -2.087  | 21.528 | 36.213 | 1.00 | 26.59 |
| ATOM | 408 | N       | ARG  | A  | 69 | -2.397  | 22.344 | 38.269 | 1.00 | 27.31 |
| ATOM | 409 | CA      | ARG  | A  | 69 | -1.330  | 23.336 | 38.101 | 1.00 | 26.13 |
| ATOM | 410 | CB      | ARG  | A  | 69 | -1.137  | 24.132 | 39.402 | 1.00 | 28.24 |
| ATOM | 411 | CG      | ARG  | A  | 69 | 0.208   | 24.842 | 39.456 | 1.00 | 33.49 |
| ATOM | 412 | CD      | ARG  | A  | 69 | 0.727   | 25.045 | 40.870 | 1.00 | 45.09 |
| ATOM | 413 | NE      | ARG  | A  | 69 | 2.100   | 24.568 | 41.036 | 1.00 | 48.71 |
| ATOM | 414 | CZ      | ARG  | A  | 69 | 3.132   | 25.001 | 40.319 | 1.00 | 51.40 |
| ATOM | 415 | NH1     | ARG  | A  | 69 | 2.961   | 25.927 | 39.384 | 1.00 | 45.02 |

**FIGURE 260**



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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |        |        |        |      |       |
|------|-----|-----|-----|---|----|--------|--------|--------|------|-------|
| ATOM | 416 | NH2 | ARG | A | 69 | 4.347  | 24.514 | 40.549 | 1.00 | 54.13 |
| ATOM | 417 | C   | ARG | A | 69 | 0.003  | 22.714 | 37.665 | 1.00 | 26.18 |
| ATOM | 418 | O   | ARG | A | 69 | 0.695  | 23.211 | 36.756 | 1.00 | 27.17 |
| ATOM | 419 | N   | GLY | A | 70 | 0.319  | 21.578 | 38.279 | 1.00 | 24.09 |
| ATOM | 420 | CA  | GLY | A | 70 | 1.568  | 20.888 | 37.993 | 1.00 | 22.34 |
| ATOM | 421 | C   | GLY | A | 70 | 1.556  | 20.175 | 36.648 | 1.00 | 22.09 |
| ATOM | 422 | O   | GLY | A | 70 | 2.579  | 19.634 | 36.252 | 1.00 | 22.14 |
| ATOM | 423 | N   | LYS | A | 71 | 0.417  | 20.179 | 35.962 | 1.00 | 18.88 |
| ATOM | 424 | CA  | LYS | A | 71 | 0.261  | 19.527 | 34.658 | 1.00 | 18.61 |
| ATOM | 425 | CB  | LYS | A | 71 | -1.192 | 19.057 | 34.499 | 1.00 | 18.52 |
| ATOM | 426 | CG  | LYS | A | 71 | -1.516 | 18.010 | 35.558 | 1.00 | 17.03 |
| ATOM | 427 | CD  | LYS | A | 71 | -2.862 | 17.421 | 35.371 | 1.00 | 16.16 |
| ATOM | 428 | CE  | LYS | A | 71 | -3.257 | 16.744 | 36.685 | 1.00 | 19.61 |
| ATOM | 429 | NZ  | LYS | A | 71 | -4.691 | 16.331 | 36.616 | 1.00 | 22.15 |
| ATOM | 430 | C   | LYS | A | 71 | 0.589  | 20.487 | 33.527 | 1.00 | 18.47 |
| ATOM | 431 | O   | LYS | A | 71 | 0.596  | 20.124 | 32.341 | 1.00 | 18.95 |
| ATOM | 432 | N   | ASN | A | 72 | 0.790  | 21.743 | 33.885 | 1.00 | 18.67 |
| ATOM | 433 | CA  | ASN | A | 72 | 1.126  | 22.757 | 32.879 | 1.00 | 19.34 |
| ATOM | 434 | CB  | ASN | A | 72 | 0.245  | 23.977 | 33.056 | 1.00 | 18.51 |
| ATOM | 435 | CG  | ASN | A | 72 | -1.206 | 23.648 | 32.847 | 1.00 | 17.81 |
| ATOM | 436 | OD1 | ASN | A | 72 | -1.576 | 23.040 | 31.838 | 1.00 | 16.74 |
| ATOM | 437 | ND2 | ASN | A | 72 | -2.035 | 24.037 | 33.801 | 1.00 | 18.58 |
| ATOM | 438 | C   | ASN | A | 72 | 2.591  | 23.158 | 32.922 | 1.00 | 18.69 |
| ATOM | 439 | O   | ASN | A | 72 | 3.075  | 23.556 | 33.981 | 1.00 | 19.55 |
| ATOM | 440 | N   | ARG | A | 73 | 3.298  | 22.983 | 31.806 | 1.00 | 19.19 |
| ATOM | 441 | CA  | ARG | A | 73 | 4.706  | 23.394 | 31.736 | 1.00 | 18.17 |
| ATOM | 442 | CB  | ARG | A | 73 | 5.277  | 23.098 | 30.351 | 1.00 | 18.40 |
| ATOM | 443 | CG  | ARG | A | 73 | 6.735  | 23.539 | 30.185 | 1.00 | 16.99 |
| ATOM | 444 | CD  | ARG | A | 73 | 7.388  | 23.053 | 28.874 | 1.00 | 16.70 |
| ATOM | 445 | NE  | ARG | A | 73 | 7.620  | 21.604 | 28.934 | 1.00 | 16.40 |
| ATOM | 446 | CZ  | ARG | A | 73 | 8.650  | 21.038 | 29.565 | 1.00 | 19.62 |
| ATOM | 447 | NH1 | ARG | A | 73 | 9.534  | 21.783 | 30.213 | 1.00 | 21.72 |
| ATOM | 448 | NH2 | ARG | A | 73 | 8.794  | 19.709 | 29.568 | 1.00 | 20.41 |
| ATOM | 449 | C   | ARG | A | 73 | 4.811  | 24.891 | 31.984 | 1.00 | 19.99 |
| ATOM | 450 | O   | ARG | A | 73 | 5.660  | 25.359 | 32.765 | 1.00 | 21.05 |
| ATOM | 451 | N   | TYR | A | 74 | 3.961  | 25.633 | 31.292 | 1.00 | 18.61 |
| ATOM | 452 | CA  | TYR | A | 74 | 3.919  | 27.081 | 31.449 | 1.00 | 18.09 |
| ATOM | 453 | CB  | TYR | A | 74 | 4.190  | 27.726 | 30.102 | 1.00 | 16.79 |
| ATOM | 454 | CG  | TYR | A | 74 | 5.560  | 27.365 | 29.541 | 1.00 | 16.34 |
| ATOM | 455 | CD1 | TYR | A | 74 | 6.722  | 27.696 | 30.196 | 1.00 | 20.25 |
| ATOM | 456 | CE1 | TYR | A | 74 | 7.971  | 27.371 | 29.649 | 1.00 | 21.10 |
| ATOM | 457 | CZ  | TYR | A | 74 | 8.034  | 26.643 | 28.469 | 1.00 | 18.00 |
| ATOM | 458 | OH  | TYR | A | 74 | 9.254  | 26.324 | 27.902 | 1.00 | 18.74 |
| ATOM | 459 | CE2 | TYR | A | 74 | 6.879  | 26.318 | 27.803 | 1.00 | 20.42 |
| ATOM | 460 | CD2 | TYR | A | 74 | 5.644  | 26.667 | 28.342 | 1.00 | 17.70 |
| ATOM | 461 | C   | TYR | A | 74 | 2.539  | 27.463 | 31.946 | 1.00 | 20.00 |
| ATOM | 462 | O   | TYR | A | 74 | 1.567  | 27.207 | 31.254 | 1.00 | 19.46 |
| ATOM | 463 | N   | ASN | A | 75 | 2.442  | 28.052 | 33.138 | 1.00 | 19.96 |
| ATOM | 464 | CA  | ASN | A | 75 | 1.125  | 28.228 | 33.729 | 1.00 | 18.71 |
| ATOM | 465 | CB  | ASN | A | 75 | 1.218  | 28.665 | 35.186 | 1.00 | 19.98 |
| ATOM | 466 | CG  | ASN | A | 75 | 1.531  | 27.534 | 36.144 | 1.00 | 28.50 |
| ATOM | 467 | OD1 | ASN | A | 75 | 1.941  | 27.798 | 37.276 | 1.00 | 41.57 |

**FIGURE 261**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 468 | ND2 | ASN | A | 75 | 1.291   | 26.291 | 35.743 | 1.00 | 34.02 |
| ATOM | 469 | C   | ASN | A | 75 | 0.300   | 29.254 | 32.975 | 1.00 | 19.22 |
| ATOM | 470 | O   | ASN | A | 75 | -0.933  | 29.328 | 33.123 | 1.00 | 19.65 |
| ATOM | 471 | N   | ASN | A | 76 | 0.970   | 30.016 | 32.122 | 1.00 | 17.60 |
| ATOM | 472 | CA  | ASN | A | 76 | 0.307   | 30.963 | 31.250 | 1.00 | 17.67 |
| ATOM | 473 | CB  | ASN | A | 76 | 1.089   | 32.267 | 31.179 | 1.00 | 19.18 |
| ATOM | 474 | CG  | ASN | A | 76 | 2.392   | 32.127 | 30.427 | 1.00 | 19.09 |
| ATOM | 475 | OD1 | ASN | A | 76 | 3.099   | 31.147 | 30.602 | 1.00 | 19.41 |
| ATOM | 476 | ND2 | ASN | A | 76 | 2.677   | 33.069 | 29.545 | 1.00 | 18.60 |
| ATOM | 477 | C   | ASN | A | 76 | -0.027  | 30.485 | 29.828 | 1.00 | 18.54 |
| ATOM | 478 | O   | ASN | A | 76 | -0.587  | 31.266 | 29.046 | 1.00 | 20.42 |
| ATOM | 479 | N   | ILE | A | 77 | 0.332   | 29.243 | 29.499 | 1.00 | 17.75 |
| ATOM | 480 | CA  | ILE | A | 77 | 0.023   | 28.679 | 28.175 | 1.00 | 16.98 |
| ATOM | 481 | CB  | ILE | A | 77 | 1.267   | 28.284 | 27.363 | 1.00 | 17.92 |
| ATOM | 482 | CG1 | ILE | A | 77 | 2.270   | 29.429 | 27.287 | 1.00 | 17.69 |
| ATOM | 483 | CD1 | ILE | A | 77 | 1.825   | 30.580 | 26.477 | 1.00 | 24.18 |
| ATOM | 484 | CG2 | ILE | A | 77 | 0.802   | 27.838 | 25.951 | 1.00 | 14.34 |
| ATOM | 485 | C   | ILE | A | 77 | -0.875  | 27.472 | 28.359 | 1.00 | 16.69 |
| ATOM | 486 | O   | ILE | A | 77 | -0.438  | 26.387 | 28.721 | 1.00 | 17.71 |
| ATOM | 487 | N   | LEU | A | 78 | -2.171  | 27.703 | 28.171 | 1.00 | 16.17 |
| ATOM | 488 | CA  | LEU | A | 78 | -3.177  | 26.760 | 28.614 | 1.00 | 15.63 |
| ATOM | 489 | CB  | LEU | A | 78 | -3.970  | 27.378 | 29.782 | 1.00 | 17.02 |
| ATOM | 490 | CG  | LEU | A | 78 | -3.103  | 27.826 | 30.952 | 1.00 | 14.20 |
| ATOM | 491 | CD1 | LEU | A | 78 | -3.971  | 28.492 | 32.013 | 1.00 | 18.34 |
| ATOM | 492 | CD2 | LEU | A | 78 | -2.351  | 26.592 | 31.530 | 1.00 | 15.97 |
| ATOM | 493 | C   | LEU | A | 78 | -4.116  | 26.521 | 27.448 | 1.00 | 16.27 |
| ATOM | 494 | O   | LEU | A | 78 | -4.338  | 27.415 | 26.640 | 1.00 | 16.45 |
| ATOM | 495 | N   | PRO | A | 79 | -4.676  | 25.319 | 27.365 | 1.00 | 15.77 |
| ATOM | 496 | CA  | PRO | A | 79 | -5.657  | 25.005 | 26.325 | 1.00 | 16.37 |
| ATOM | 497 | CB  | PRO | A | 79 | -5.825  | 23.494 | 26.465 | 1.00 | 15.52 |
| ATOM | 498 | CG  | PRO | A | 79 | -5.511  | 23.196 | 27.896 | 1.00 | 16.91 |
| ATOM | 499 | CD  | PRO | A | 79 | -4.409  | 24.186 | 28.269 | 1.00 | 16.37 |
| ATOM | 500 | C   | PRO | A | 79 | -7.001  | 25.658 | 26.657 | 1.00 | 15.83 |
| ATOM | 501 | O   | PRO | A | 79 | -7.397  | 25.687 | 27.824 | 1.00 | 16.64 |
| ATOM | 502 | N   | TYR | A | 80 | -7.668  | 26.191 | 25.639 | 1.00 | 17.68 |
| ATOM | 503 | CA  | TYR | A | 80 | -9.073  | 26.594 | 25.776 | 1.00 | 16.66 |
| ATOM | 504 | CB  | TYR | A | 80 | -9.571  | 27.131 | 24.426 | 1.00 | 17.47 |
| ATOM | 505 | CG  | TYR | A | 80 | -8.862  | 28.405 | 23.974 | 1.00 | 18.71 |
| ATOM | 506 | CD1 | TYR | A | 80 | -8.661  | 29.469 | 24.864 | 1.00 | 21.72 |
| ATOM | 507 | CE1 | TYR | A | 80 | -8.008  | 30.612 | 24.458 | 1.00 | 18.65 |
| ATOM | 508 | CZ  | TYR | A | 80 | -7.552  | 30.728 | 23.163 | 1.00 | 18.69 |
| ATOM | 509 | OH  | TYR | A | 80 | -6.951  | 31.901 | 22.794 | 1.00 | 19.69 |
| ATOM | 510 | CE2 | TYR | A | 80 | -7.730  | 29.709 | 22.252 | 1.00 | 19.15 |
| ATOM | 511 | CD2 | TYR | A | 80 | -8.363  | 28.532 | 22.676 | 1.00 | 18.51 |
| ATOM | 512 | C   | TYR | A | 80 | -9.944  | 25.419 | 26.190 | 1.00 | 17.71 |
| ATOM | 513 | O   | TYR | A | 80 | -9.835  | 24.326 | 25.641 | 1.00 | 18.31 |
| ATOM | 514 | N   | ASP | A | 81 | -10.884 | 25.656 | 27.098 | 1.00 | 17.08 |
| ATOM | 515 | CA  | ASP | A | 81 | -11.881 | 24.660 | 27.444 | 1.00 | 17.40 |
| ATOM | 516 | CB  | ASP | A | 81 | -12.929 | 25.314 | 28.332 | 1.00 | 18.47 |
| ATOM | 517 | CG  | ASP | A | 81 | -12.361 | 25.790 | 29.649 | 1.00 | 22.96 |
| ATOM | 518 | OD1 | ASP | A | 81 | -11.447 | 25.148 | 30.229 | 1.00 | 20.84 |
| ATOM | 519 | OD2 | ASP | A | 81 | -12.841 | 26.794 | 30.205 | 1.00 | 19.85 |

**FIGURE 262**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 520 | C   | ASP | A | 81 | -12.568 | 24.065 | 26.215 | 1.00 | 16.40 |
| ATOM | 521 | O   | ASP | A | 81 | -12.790 | 22.845 | 26.175 | 1.00 | 18.31 |
| ATOM | 522 | N   | ALA | A | 82 | -12.901 | 24.923 | 25.248 | 1.00 | 18.79 |
| ATOM | 523 | CA  | ALA | A | 82 | -13.714 | 24.544 | 24.096 | 1.00 | 21.05 |
| ATOM | 524 | CB  | ALA | A | 82 | -14.082 | 25.787 | 23.284 | 1.00 | 22.15 |
| ATOM | 525 | C   | ALA | A | 82 | -13.065 | 23.500 | 23.194 | 1.00 | 20.96 |
| ATOM | 526 | O   | ALA | A | 82 | -13.763 | 22.798 | 22.459 | 1.00 | 19.35 |
| ATOM | 527 | N   | THR | A | 83 | -11.730 | 23.441 | 23.203 | 1.00 | 18.07 |
| ATOM | 528 | CA  | THR | A | 83 | -11.029 | 22.560 | 22.274 | 1.00 | 20.13 |
| ATOM | 529 | CB  | THR | A | 83 | -10.260 | 23.375 | 21.204 | 1.00 | 21.39 |
| ATOM | 530 | OG1 | THR | A | 83 | -9.399  | 24.306 | 21.888 | 1.00 | 20.87 |
| ATOM | 531 | CG2 | THR | A | 83 | -11.215 | 24.257 | 20.373 | 1.00 | 22.64 |
| ATOM | 532 | C   | THR | A | 83 | -10.015 | 21.647 | 22.962 | 1.00 | 19.11 |
| ATOM | 533 | O   | THR | A | 83 | -9.241  | 21.027 | 22.255 | 1.00 | 18.63 |
| ATOM | 534 | N   | ARG | A | 84 | -10.008 | 21.543 | 24.292 | 1.00 | 16.72 |
| ATOM | 535 | CA  | ARG | A | 84 | -8.994  | 20.752 | 24.973 | 1.00 | 18.30 |
| ATOM | 536 | CB  | ARG | A | 84 | -8.977  | 21.025 | 26.481 | 1.00 | 20.17 |
| ATOM | 537 | CG  | ARG | A | 84 | -10.132 | 20.412 | 27.255 | 1.00 | 21.69 |
| ATOM | 538 | CD  | ARG | A | 84 | -10.152 | 20.875 | 28.716 | 1.00 | 21.07 |
| ATOM | 539 | NE  | ARG | A | 84 | -11.233 | 20.227 | 29.455 | 1.00 | 18.74 |
| ATOM | 540 | CZ  | ARG | A | 84 | -11.068 | 19.171 | 30.257 | 1.00 | 17.05 |
| ATOM | 541 | NH1 | ARG | A | 84 | -9.857  | 18.640 | 30.407 | 1.00 | 17.98 |
| ATOM | 542 | NH2 | ARG | A | 84 | -12.125 | 18.639 | 30.884 | 1.00 | 17.21 |
| ATOM | 543 | C   | ARG | A | 84 | -9.207  | 19.276 | 24.702 | 1.00 | 18.78 |
| ATOM | 544 | O   | ARG | A | 84 | -10.348 | 18.839 | 24.517 | 1.00 | 19.49 |
| ATOM | 545 | N   | VAL | A | 85 | -8.108  | 18.538 | 24.710 | 1.00 | 17.44 |
| ATOM | 546 | CA  | VAL | A | 85 | -8.130  | 17.081 | 24.614 | 1.00 | 17.40 |
| ATOM | 547 | CB  | VAL | A | 85 | -6.799  | 16.539 | 24.064 | 1.00 | 18.13 |
| ATOM | 548 | CG1 | VAL | A | 85 | -6.897  | 15.001 | 23.926 | 1.00 | 17.98 |
| ATOM | 549 | CG2 | VAL | A | 85 | -6.493  | 17.177 | 22.686 | 1.00 | 19.36 |
| ATOM | 550 | C   | VAL | A | 85 | -8.371  | 16.488 | 26.003 | 1.00 | 18.79 |
| ATOM | 551 | O   | VAL | A | 85 | -7.719  | 16.869 | 26.976 | 1.00 | 19.65 |
| ATOM | 552 | N   | LYS | A | 86 | -9.315  | 15.555 | 26.094 | 1.00 | 18.68 |
| ATOM | 553 | CA  | LYS | A | 86 | -9.613  | 14.946 | 27.396 | 1.00 | 17.68 |
| ATOM | 554 | CB  | LYS | A | 86 | -11.137 | 14.942 | 27.623 | 1.00 | 18.74 |
| ATOM | 555 | CG  | LYS | A | 86 | -11.672 | 16.355 | 27.728 | 1.00 | 22.75 |
| ATOM | 556 | CD  | LYS | A | 86 | -13.167 | 16.435 | 27.837 | 1.00 | 27.00 |
| ATOM | 557 | CE  | LYS | A | 86 | -13.540 | 17.906 | 27.691 | 1.00 | 30.36 |
| ATOM | 558 | NZ  | LYS | A | 86 | -14.942 | 18.132 | 27.228 | 1.00 | 34.08 |
| ATOM | 559 | C   | LYS | A | 86 | -9.118  | 13.517 | 27.445 | 1.00 | 19.75 |
| ATOM | 560 | O   | LYS | A | 86 | -9.357  | 12.766 | 26.489 | 1.00 | 22.00 |
| ATOM | 561 | N   | LEU | A | 87 | -8.443  | 13.188 | 28.544 | 1.00 | 19.49 |
| ATOM | 562 | CA  | LEU | A | 87 | -8.007  | 11.819 | 28.836 | 1.00 | 21.14 |
| ATOM | 563 | CB  | LEU | A | 87 | -6.883  | 11.849 | 29.871 | 1.00 | 20.71 |
| ATOM | 564 | CG  | LEU | A | 87 | -5.611  | 12.606 | 29.453 | 1.00 | 24.00 |
| ATOM | 565 | CD1 | LEU | A | 87 | -4.671  | 12.651 | 30.634 | 1.00 | 23.82 |
| ATOM | 566 | CD2 | LEU | A | 87 | -4.924  | 11.964 | 28.229 | 1.00 | 22.65 |
| ATOM | 567 | C   | LEU | A | 87 | -9.214  | 11.092 | 29.426 | 1.00 | 21.83 |
| ATOM | 568 | O   | LEU | A | 87 | -10.077 | 11.716 | 30.069 | 1.00 | 21.33 |
| ATOM | 569 | N   | SER | A | 88 | -9.278  | 9.777  | 29.239 | 1.00 | 22.50 |
| ATOM | 570 | CA  | SER | A | 88 | -10.267 | 9.015  | 30.030 | 1.00 | 27.20 |
| ATOM | 571 | CB  | SER | A | 88 | -10.199 | 7.517  | 29.746 | 1.00 | 26.15 |

**FIGURE 263**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |    |         |        |        |      |       |
|------|-----|-----|-----|---|----|---------|--------|--------|------|-------|
| ATOM | 572 | OG  | SER | A | 88 | -8.930  | 6.992  | 30.099 | 1.00 | 27.44 |
| ATOM | 573 | C   | SER | A | 88 | -10.120 | 9.264  | 31.527 | 1.00 | 29.45 |
| ATOM | 574 | O   | SER | A | 88 | -9.021  | 9.477  | 32.035 | 1.00 | 28.78 |
| ATOM | 575 | N   | ASN | A | 89 | -11.244 | 9.263  | 32.234 | 1.00 | 33.66 |
| ATOM | 576 | CA  | ASN | A | 89 | -11.240 | 9.331  | 33.697 | 1.00 | 38.59 |
| ATOM | 577 | CB  | ASN | A | 89 | -12.675 | 9.420  | 34.228 | 1.00 | 40.00 |
| ATOM | 578 | CG  | ASN | A | 89 | -13.511 | 10.437 | 33.472 | 1.00 | 44.74 |
| ATOM | 579 | OD1 | ASN | A | 89 | -13.097 | 10.948 | 32.425 | 1.00 | 50.87 |
| ATOM | 580 | ND2 | ASN | A | 89 | -14.702 | 10.725 | 33.990 | 1.00 | 48.81 |
| ATOM | 581 | C   | ASN | A | 89 | -10.510 | 8.180  | 34.383 | 1.00 | 39.26 |
| ATOM | 582 | O   | ASN | A | 89 | -10.637 | 7.018  | 33.977 | 1.00 | 40.17 |
| ATOM | 583 | N   | VAL | A | 90 | -9.750  | 8.521  | 35.420 | 1.00 | 39.03 |
| ATOM | 584 | CA  | VAL | A | 90 | -9.059  | 7.551  | 36.267 | 1.00 | 39.07 |
| ATOM | 585 | CB  | VAL | A | 90 | -7.579  | 7.933  | 36.450 | 1.00 | 39.43 |
| ATOM | 586 | CG1 | VAL | A | 90 | -6.890  | 7.053  | 37.502 | 1.00 | 39.89 |
| ATOM | 587 | CG2 | VAL | A | 90 | -6.848  | 7.840  | 35.114 | 1.00 | 39.94 |
| ATOM | 588 | C   | VAL | A | 90 | -9.724  | 7.437  | 37.641 | 1.00 | 39.53 |
| ATOM | 589 | O   | VAL | A | 90 | -10.029 | 8.446  | 38.277 | 1.00 | 39.69 |
| ATOM | 590 | N   | CYS | A | 95 | -10.123 | 15.551 | 38.257 | 1.00 | 32.20 |
| ATOM | 591 | CA  | CYS | A | 95 | -9.274  | 16.239 | 37.274 | 1.00 | 31.56 |
| ATOM | 592 | CB  | CYS | A | 95 | -8.436  | 17.341 | 37.923 | 1.00 | 32.45 |
| ATOM | 593 | SG  | CYS | A | 95 | -9.470  | 18.646 | 38.623 | 1.00 | 39.21 |
| ATOM | 594 | C   | CYS | A | 95 | -8.351  | 15.296 | 36.529 | 1.00 | 29.09 |
| ATOM | 595 | O   | CYS | A | 95 | -7.399  | 15.760 | 35.888 | 1.00 | 28.47 |
| ATOM | 596 | N   | SER | A | 96 | -8.624  | 13.992 | 36.611 | 1.00 | 25.31 |
| ATOM | 597 | CA  | SER | A | 96 | -7.816  | 13.009 | 35.891 | 1.00 | 26.34 |
| ATOM | 598 | CB  | SER | A | 96 | -8.104  | 11.576 | 36.380 | 1.00 | 26.13 |
| ATOM | 599 | OG  | SER | A | 96 | -9.450  | 11.210 | 36.131 | 1.00 | 28.38 |
| ATOM | 600 | C   | SER | A | 96 | -7.857  | 13.149 | 34.365 | 1.00 | 24.83 |
| ATOM | 601 | O   | SER | A | 96 | -6.970  | 12.661 | 33.640 | 1.00 | 25.70 |
| ATOM | 602 | N   | ASP | A | 97 | -8.863  | 13.860 | 33.873 | 1.00 | 23.60 |
| ATOM | 603 | CA  | ASP | A | 97 | -9.022  | 14.004 | 32.432 | 1.00 | 23.00 |
| ATOM | 604 | CB  | ASP | A | 97 | -10.486 | 14.244 | 32.031 | 1.00 | 23.06 |
| ATOM | 605 | CG  | ASP | A | 97 | -10.939 | 15.704 | 32.178 | 1.00 | 25.86 |
| ATOM | 606 | OD1 | ASP | A | 97 | -10.131 | 16.559 | 32.575 | 1.00 | 23.58 |
| ATOM | 607 | OD2 | ASP | A | 97 | -12.113 | 16.073 | 31.926 | 1.00 | 27.66 |
| ATOM | 608 | C   | ASP | A | 97 | -8.085  | 15.005 | 31.779 | 1.00 | 20.67 |
| ATOM | 609 | O   | ASP | A | 97 | -8.055  | 15.123 | 30.548 | 1.00 | 21.87 |
| ATOM | 610 | N   | TYR | A | 98 | -7.333  | 15.746 | 32.581 | 1.00 | 19.60 |
| ATOM | 611 | CA  | TYR | A | 98 | -6.691  | 16.926 | 32.030 | 1.00 | 18.52 |
| ATOM | 612 | CB  | TYR | A | 98 | -6.520  | 18.003 | 33.104 | 1.00 | 18.03 |
| ATOM | 613 | CG  | TYR | A | 98 | -5.822  | 19.205 | 32.517 | 1.00 | 19.58 |
| ATOM | 614 | CD1 | TYR | A | 98 | -6.534  | 20.124 | 31.746 | 1.00 | 21.57 |
| ATOM | 615 | CE1 | TYR | A | 98 | -5.904  | 21.216 | 31.192 | 1.00 | 16.87 |
| ATOM | 616 | CZ  | TYR | A | 98 | -4.536  | 21.375 | 31.389 | 1.00 | 16.22 |
| ATOM | 617 | OH  | TYR | A | 98 | -3.906  | 22.447 | 30.797 | 1.00 | 18.85 |
| ATOM | 618 | CE2 | TYR | A | 98 | -3.803  | 20.475 | 32.138 | 1.00 | 17.86 |
| ATOM | 619 | CD2 | TYR | A | 98 | -4.445  | 19.385 | 32.694 | 1.00 | 19.81 |
| ATOM | 620 | C   | TYR | A | 98 | -5.338  | 16.650 | 31.410 | 1.00 | 16.72 |
| ATOM | 621 | O   | TYR | A | 98 | -4.485  | 16.025 | 32.040 | 1.00 | 19.70 |
| ATOM | 622 | N   | ILE | A | 99 | -5.137  | 17.179 | 30.199 | 1.00 | 15.99 |
| ATOM | 623 | CA  | ILE | A | 99 | -3.773  | 17.307 | 29.653 | 1.00 | 15.12 |

**FIGURE 264**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |         |        |        |      |       |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 624 | CB  | ILE | A | 99  | -3.485  | 16.142 | 28.679 | 1.00 | 16.27 |
| ATOM | 625 | CG1 | ILE | A | 99  | -2.013  | 16.171 | 28.227 | 1.00 | 13.41 |
| ATOM | 626 | CD1 | ILE | A | 99  | -1.501  | 14.952 | 27.413 | 1.00 | 15.15 |
| ATOM | 627 | CG2 | ILE | A | 99  | -4.516  | 16.099 | 27.536 | 1.00 | 18.41 |
| ATOM | 628 | C   | ILE | A | 99  | -3.730  | 18.654 | 28.924 | 1.00 | 14.61 |
| ATOM | 629 | O   | ILE | A | 99  | -4.754  | 19.134 | 28.452 | 1.00 | 14.64 |
| ATOM | 630 | N   | ASN | A | 100 | -2.549  | 19.246 | 28.845 | 1.00 | 13.96 |
| ATOM | 631 | CA  | ASN | A | 100 | -2.381  | 20.522 | 28.162 | 1.00 | 15.20 |
| ATOM | 632 | CB  | ASN | A | 100 | -1.218  | 21.330 | 28.763 | 1.00 | 15.09 |
| ATOM | 633 | CG  | ASN | A | 100 | -1.167  | 22.726 | 28.214 | 1.00 | 15.71 |
| ATOM | 634 | OD1 | ASN | A | 100 | -1.374  | 22.917 | 27.020 | 1.00 | 16.88 |
| ATOM | 635 | ND2 | ASN | A | 100 | -0.873  | 23.698 | 29.060 | 1.00 | 15.13 |
| ATOM | 636 | C   | ASN | A | 100 | -2.184  | 20.228 | 26.679 | 1.00 | 14.05 |
| ATOM | 637 | O   | ASN | A | 100 | -1.068  | 20.052 | 26.188 | 1.00 | 15.61 |
| ATOM | 638 | N   | ALA | A | 101 | -3.321  | 20.129 | 26.011 | 1.00 | 14.18 |
| ATOM | 639 | CA  | ALA | A | 101 | -3.342  | 19.806 | 24.587 | 1.00 | 14.86 |
| ATOM | 640 | CB  | ALA | A | 101 | -3.238  | 18.306 | 24.435 | 1.00 | 14.35 |
| ATOM | 641 | C   | ALA | A | 101 | -4.665  | 20.251 | 24.018 | 1.00 | 15.17 |
| ATOM | 642 | O   | ALA | A | 101 | -5.669  | 20.248 | 24.743 | 1.00 | 14.69 |
| ATOM | 643 | N   | SER | A | 102 | -4.679  | 20.523 | 22.708 | 1.00 | 15.50 |
| ATOM | 644 | CA  | SER | A | 102 | -5.810  | 21.159 | 22.047 | 1.00 | 15.05 |
| ATOM | 645 | CB  | SER | A | 102 | -5.471  | 22.629 | 21.759 | 1.00 | 15.31 |
| ATOM | 646 | OG  | SER | A | 102 | -5.151  | 23.291 | 22.969 | 1.00 | 15.76 |
| ATOM | 647 | C   | SER | A | 102 | -6.060  | 20.499 | 20.687 | 1.00 | 14.47 |
| ATOM | 648 | O   | SER | A | 102 | -5.122  | 20.253 | 19.962 | 1.00 | 16.41 |
| ATOM | 649 | N   | TYR | A | 103 | -7.315  | 20.273 | 20.310 | 1.00 | 14.11 |
| ATOM | 650 | CA  | TYR | A | 103 | -7.625  | 19.700 | 18.994 | 1.00 | 16.15 |
| ATOM | 651 | CB  | TYR | A | 103 | -9.064  | 19.128 | 18.983 | 1.00 | 15.58 |
| ATOM | 652 | CG  | TYR | A | 103 | -9.226  | 17.837 | 19.738 | 1.00 | 17.69 |
| ATOM | 653 | CD1 | TYR | A | 103 | -8.530  | 16.696 | 19.331 | 1.00 | 21.85 |
| ATOM | 654 | CE1 | TYR | A | 103 | -8.681  | 15.485 | 20.004 | 1.00 | 18.09 |
| ATOM | 655 | CZ  | TYR | A | 103 | -9.560  | 15.417 | 21.070 | 1.00 | 23.34 |
| ATOM | 656 | OH  | TYR | A | 103 | -9.763  | 14.235 | 21.749 | 1.00 | 25.07 |
| ATOM | 657 | CE2 | TYR | A | 103 | -10.281 | 16.527 | 21.482 | 1.00 | 22.71 |
| ATOM | 658 | CD2 | TYR | A | 103 | -10.123 | 17.724 | 20.808 | 1.00 | 19.56 |
| ATOM | 659 | C   | TYR | A | 103 | -7.606  | 20.816 | 17.968 | 1.00 | 17.25 |
| ATOM | 660 | O   | TYR | A | 103 | -8.067  | 21.930 | 18.244 | 1.00 | 18.82 |
| ATOM | 661 | N   | ILE | A | 104 | -7.125  | 20.470 | 16.779 | 1.00 | 16.96 |
| ATOM | 662 | CA  | ILE | A | 104 | -7.227  | 21.292 | 15.577 | 1.00 | 17.89 |
| ATOM | 663 | CB  | ILE | A | 104 | -5.810  | 21.550 | 15.040 | 1.00 | 18.29 |
| ATOM | 664 | CG1 | ILE | A | 104 | -4.887  | 21.993 | 16.154 | 1.00 | 19.03 |
| ATOM | 665 | CD1 | ILE | A | 104 | -5.247  | 23.333 | 16.819 | 1.00 | 21.70 |
| ATOM | 666 | CG2 | ILE | A | 104 | -5.845  | 22.465 | 13.784 | 1.00 | 22.08 |
| ATOM | 667 | C   | ILE | A | 104 | -8.013  | 20.483 | 14.547 | 1.00 | 20.87 |
| ATOM | 668 | O   | ILE | A | 104 | -7.582  | 19.407 | 14.121 | 1.00 | 20.90 |
| ATOM | 669 | N   | PRO | A | 105 | -9.188  | 20.966 | 14.154 | 1.00 | 21.39 |
| ATOM | 670 | CA  | PRO | A | 105 | -9.980  | 20.233 | 13.162 | 1.00 | 20.64 |
| ATOM | 671 | CB  | PRO | A | 105 | -11.348 | 20.918 | 13.214 | 1.00 | 21.14 |
| ATOM | 672 | CG  | PRO | A | 105 | -11.064 | 22.320 | 13.696 | 1.00 | 25.38 |
| ATOM | 673 | CD  | PRO | A | 105 | -9.836  | 22.219 | 14.596 | 1.00 | 22.10 |
| ATOM | 674 | C   | PRO | A | 105 | -9.346  | 20.426 | 11.786 | 1.00 | 20.86 |
| ATOM | 675 | O   | PRO | A | 105 | -8.621  | 21.420 | 11.579 | 1.00 | 22.00 |

**FIGURE 265**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |         |        |        |      |       |
|------|-----|-----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 676 | N   | GLY | A | 106 | -9.603  | 19.487 | 10.872 | 1.00 | 20.78 |
| ATOM | 677 | CA  | GLY | A | 106 | -9.258  | 19.643 | 9.472  | 1.00 | 23.04 |
| ATOM | 678 | C   | GLY | A | 106 | -10.329 | 20.332 | 8.646  | 1.00 | 25.39 |
| ATOM | 679 | O   | GLY | A | 106 | -11.440 | 20.586 | 9.124  | 1.00 | 24.34 |
| ATOM | 680 | N   | ASN | A | 107 | -10.001 | 20.603 | 7.386  | 1.00 | 27.36 |
| ATOM | 681 | CA  | ASN | A | 107 | -10.986 | 21.163 | 6.458  | 1.00 | 29.29 |
| ATOM | 682 | CB  | ASN | A | 107 | -10.336 | 21.579 | 5.142  | 1.00 | 31.82 |
| ATOM | 683 | CG  | ASN | A | 107 | -9.436  | 22.795 | 5.291  | 1.00 | 34.51 |
| ATOM | 684 | OD1 | ASN | A | 107 | -8.306  | 22.792 | 4.798  | 1.00 | 43.42 |
| ATOM | 685 | ND2 | ASN | A | 107 | -9.917  | 23.824 | 5.984  | 1.00 | 40.29 |
| ATOM | 686 | C   | ASN | A | 107 | -12.080 | 20.168 | 6.153  | 1.00 | 28.84 |
| ATOM | 687 | O   | ASN | A | 107 | -13.182 | 20.560 | 5.772  | 1.00 | 29.29 |
| ATOM | 688 | N   | ASN | A | 108 | -11.776 | 18.881 | 6.300  | 1.00 | 27.42 |
| ATOM | 689 | CA  | ASN | A | 108 | -12.716 | 17.847 | 5.886  | 1.00 | 28.42 |
| ATOM | 690 | CB  | ASN | A | 108 | -12.020 | 16.861 | 4.947  | 1.00 | 29.82 |
| ATOM | 691 | CG  | ASN | A | 108 | -11.769 | 17.438 | 3.570  | 1.00 | 33.34 |
| ATOM | 692 | OD1 | ASN | A | 108 | -10.623 | 17.630 | 3.158  | 1.00 | 39.32 |
| ATOM | 693 | ND2 | ASN | A | 108 | -12.846 | 17.710 | 2.843  | 1.00 | 37.81 |
| ATOM | 694 | C   | ASN | A | 108 | -13.325 | 17.065 | 7.052  | 1.00 | 27.69 |
| ATOM | 695 | O   | ASN | A | 108 | -14.371 | 16.440 | 6.895  | 1.00 | 28.98 |
| ATOM | 696 | N   | PHE | A | 109 | -12.665 | 17.078 | 8.206  | 1.00 | 24.03 |
| ATOM | 697 | CA  | PHE | A | 109 | -13.114 | 16.259 | 9.339  | 1.00 | 21.78 |
| ATOM | 698 | CB  | PHE | A | 109 | -12.718 | 14.795 | 9.081  | 1.00 | 20.51 |
| ATOM | 699 | CG  | PHE | A | 109 | -13.564 | 13.780 | 9.830  | 1.00 | 21.38 |
| ATOM | 700 | CD1 | PHE | A | 109 | -13.061 | 13.110 | 10.936 | 1.00 | 21.50 |
| ATOM | 701 | CE1 | PHE | A | 109 | -13.823 | 12.180 | 11.626 | 1.00 | 24.12 |
| ATOM | 702 | CZ  | PHE | A | 109 | -15.129 | 11.909 | 11.208 | 1.00 | 25.45 |
| ATOM | 703 | CE2 | PHE | A | 109 | -15.641 | 12.561 | 10.113 | 1.00 | 21.35 |
| ATOM | 704 | CD2 | PHE | A | 109 | -14.866 | 13.493 | 9.421  | 1.00 | 18.54 |
| ATOM | 705 | C   | PHE | A | 109 | -12.452 | 16.764 | 10.612 | 1.00 | 22.13 |
| ATOM | 706 | O   | PHE | A | 109 | -11.412 | 17.437 | 10.545 | 1.00 | 21.08 |
| ATOM | 707 | N   | ARG | A | 110 | -13.013 | 16.358 | 11.752 | 1.00 | 19.50 |
| ATOM | 708 | CA  | ARG | A | 110 | -12.523 | 16.785 | 13.054 | 1.00 | 21.56 |
| ATOM | 709 | CB  | ARG | A | 110 | -13.472 | 16.347 | 14.168 | 1.00 | 22.46 |
| ATOM | 710 | CG  | ARG | A | 110 | -13.476 | 14.851 | 14.413 | 1.00 | 24.80 |
| ATOM | 711 | CD  | ARG | A | 110 | -14.802 | 14.225 | 14.822 | 1.00 | 32.72 |
| ATOM | 712 | NE  | ARG | A | 110 | -15.236 | 14.643 | 16.150 | 1.00 | 39.42 |
| ATOM | 713 | CZ  | ARG | A | 110 | -15.044 | 13.914 | 17.243 | 1.00 | 43.17 |
| ATOM | 714 | NH1 | ARG | A | 110 | -14.400 | 12.750 | 17.162 | 1.00 | 42.56 |
| ATOM | 715 | NH2 | ARG | A | 110 | -15.474 | 14.358 | 18.418 | 1.00 | 43.79 |
| ATOM | 716 | C   | ARG | A | 110 | -11.118 | 16.239 | 13.310 | 1.00 | 20.39 |
| ATOM | 717 | O   | ARG | A | 110 | -10.729 | 15.220 | 12.746 | 1.00 | 21.44 |
| ATOM | 718 | N   | ARG | A | 111 | -10.436 | 16.843 | 14.273 | 1.00 | 20.63 |
| ATOM | 719 | CA  | ARG | A | 111 | -9.259  | 16.240 | 14.885 | 1.00 | 21.26 |
| ATOM | 720 | CB  | ARG | A | 111 | -9.651  | 15.008 | 15.728 | 1.00 | 20.41 |
| ATOM | 721 | CG  | ARG | A | 111 | -10.650 | 15.324 | 16.827 | 1.00 | 21.47 |
| ATOM | 722 | CD  | ARG | A | 111 | -10.936 | 14.151 | 17.754 | 1.00 | 21.72 |
| ATOM | 723 | NE  | ARG | A | 111 | -11.920 | 14.585 | 18.729 | 1.00 | 22.21 |
| ATOM | 724 | CZ  | ARG | A | 111 | -12.269 | 13.928 | 19.825 | 1.00 | 27.64 |
| ATOM | 725 | NH1 | ARG | A | 111 | -11.713 | 12.759 | 20.119 | 1.00 | 30.92 |
| ATOM | 726 | NH2 | ARG | A | 111 | -13.175 | 14.456 | 20.633 | 1.00 | 26.56 |
| ATOM | 727 | C   | ARG | A | 111 | -8.161  | 15.872 | 13.914 | 1.00 | 20.16 |

**FIGURE 266**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 728 | O   | ARG | A | 111 | -7.612 | 14.761 | 13.972 | 1.00 | 21.20 |
| ATOM | 729 | N   | GLU | A | 112 | -7.777 | 16.801 | 13.043 | 1.00 | 18.71 |
| ATOM | 730 | CA  | GLU | A | 112 | -6.651 | 16.499 | 12.179 | 1.00 | 17.48 |
| ATOM | 731 | CB  | GLU | A | 112 | -6.632 | 17.426 | 10.954 | 1.00 | 18.75 |
| ATOM | 732 | CG  | GLU | A | 112 | -5.441 | 17.169 | 10.049 | 1.00 | 16.97 |
| ATOM | 733 | CD  | GLU | A | 112 | -5.437 | 18.043 | 8.809  | 1.00 | 27.96 |
| ATOM | 734 | OE1 | GLU | A | 112 | -4.889 | 17.541 | 7.805  | 1.00 | 25.67 |
| ATOM | 735 | OE2 | GLU | A | 112 | -5.919 | 19.209 | 8.860  | 1.00 | 25.41 |
| ATOM | 736 | C   | GLU | A | 112 | -5.307 | 16.580 | 12.906 | 1.00 | 16.93 |
| ATOM | 737 | O   | GLU | A | 112 | -4.421 | 15.771 | 12.615 | 1.00 | 17.02 |
| ATOM | 738 | N   | TYR | A | 113 | -5.168 | 17.526 | 13.834 | 1.00 | 16.48 |
| ATOM | 739 | CA  | TYR | A | 113 | -3.964 | 17.632 | 14.673 | 1.00 | 17.06 |
| ATOM | 740 | CB  | TYR | A | 113 | -3.168 | 18.898 | 14.387 | 1.00 | 15.83 |
| ATOM | 741 | CG  | TYR | A | 113 | -2.779 | 19.127 | 12.955 | 1.00 | 18.99 |
| ATOM | 742 | CD1 | TYR | A | 113 | -3.606 | 19.884 | 12.148 | 1.00 | 22.98 |
| ATOM | 743 | CE1 | TYR | A | 113 | -3.290 | 20.157 | 10.850 | 1.00 | 24.83 |
| ATOM | 744 | CZ  | TYR | A | 113 | -2.089 | 19.709 | 10.356 | 1.00 | 22.77 |
| ATOM | 745 | OH  | TYR | A | 113 | -1.838 | 20.017 | 9.035  | 1.00 | 28.70 |
| ATOM | 746 | CE2 | TYR | A | 113 | -1.233 | 18.945 | 11.118 | 1.00 | 22.82 |
| ATOM | 747 | CD2 | TYR | A | 113 | -1.570 | 18.678 | 12.457 | 1.00 | 24.11 |
| ATOM | 748 | C   | TYR | A | 113 | -4.327 | 17.701 | 16.163 | 1.00 | 14.55 |
| ATOM | 749 | O   | TYR | A | 113 | -5.445 | 18.039 | 16.533 | 1.00 | 16.23 |
| ATOM | 750 | N   | ILE | A | 114 | -3.439 | 17.251 | 17.029 | 1.00 | 13.11 |
| ATOM | 751 | CA  | ILE | A | 114 | -3.500 | 17.610 | 18.439 | 1.00 | 13.46 |
| ATOM | 752 | CB  | ILE | A | 114 | -3.501 | 16.340 | 19.331 | 1.00 | 13.02 |
| ATOM | 753 | CG1 | ILE | A | 114 | -4.859 | 15.643 | 19.231 | 1.00 | 15.50 |
| ATOM | 754 | CD1 | ILE | A | 114 | -4.796 | 14.175 | 19.736 | 1.00 | 17.84 |
| ATOM | 755 | CG2 | ILE | A | 114 | -3.233 | 16.721 | 20.803 | 1.00 | 15.76 |
| ATOM | 756 | C   | ILE | A | 114 | -2.239 | 18.421 | 18.708 | 1.00 | 15.12 |
| ATOM | 757 | O   | ILE | A | 114 | -1.146 | 17.951 | 18.448 | 1.00 | 16.55 |
| ATOM | 758 | N   | VAL | A | 115 | -2.407 | 19.636 | 19.215 | 1.00 | 15.68 |
| ATOM | 759 | CA  | VAL | A | 115 | -1.262 | 20.440 | 19.619 | 1.00 | 14.96 |
| ATOM | 760 | CB  | VAL | A | 115 | -1.499 | 21.899 | 19.277 | 1.00 | 15.98 |
| ATOM | 761 | CG1 | VAL | A | 115 | -0.446 | 22.789 | 19.895 | 1.00 | 18.83 |
| ATOM | 762 | CG2 | VAL | A | 115 | -1.501 | 22.011 | 17.767 | 1.00 | 19.14 |
| ATOM | 763 | C   | VAL | A | 115 | -1.078 | 20.282 | 21.114 | 1.00 | 15.79 |
| ATOM | 764 | O   | VAL | A | 115 | -2.039 | 20.346 | 21.880 | 1.00 | 15.38 |
| ATOM | 765 | N   | THR | A | 116 | 0.163  | 20.062 | 21.541 | 1.00 | 14.14 |
| ATOM | 766 | CA  | THR | A | 116 | 0.399  | 19.938 | 22.966 | 1.00 | 15.23 |
| ATOM | 767 | CB  | THR | A | 116 | 0.267  | 18.421 | 23.362 | 1.00 | 15.94 |
| ATOM | 768 | OG1 | THR | A | 116 | 0.282  | 18.318 | 24.792 | 1.00 | 16.48 |
| ATOM | 769 | CG2 | THR | A | 116 | 1.492  | 17.619 | 22.906 | 1.00 | 20.42 |
| ATOM | 770 | C   | THR | A | 116 | 1.737  | 20.589 | 23.403 | 1.00 | 14.47 |
| ATOM | 771 | O   | THR | A | 116 | 2.563  | 20.939 | 22.583 | 1.00 | 17.79 |
| ATOM | 772 | N   | GLN | A | 117 | 1.924  | 20.762 | 24.706 | 1.00 | 16.11 |
| ATOM | 773 | CA  | GLN | A | 117 | 3.181  | 21.248 | 25.251 | 1.00 | 15.39 |
| ATOM | 774 | CB  | GLN | A | 117 | 2.975  | 21.710 | 26.716 | 1.00 | 14.51 |
| ATOM | 775 | CG  | GLN | A | 117 | 2.597  | 20.569 | 27.659 | 1.00 | 15.32 |
| ATOM | 776 | CD  | GLN | A | 117 | 2.327  | 21.017 | 29.072 | 1.00 | 16.29 |
| ATOM | 777 | OE1 | GLN | A | 117 | 2.162  | 22.202 | 29.329 | 1.00 | 17.89 |
| ATOM | 778 | NE2 | GLN | A | 117 | 2.265  | 20.073 | 29.987 | 1.00 | 15.78 |
| ATOM | 779 | C   | GLN | A | 117 | 4.208  | 20.143 | 25.228 | 1.00 | 16.18 |

**FIGURE 267**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 780 | O   | GLN | A | 117 | 3.895  | 18.970 | 25.110 | 1.00 | 16.55 |
| ATOM | 781 | N   | GLY | A | 118 | 5.469  | 20.517 | 25.375 | 1.00 | 16.92 |
| ATOM | 782 | CA  | GLY | A | 118 | 6.470  | 19.495 | 25.606 | 1.00 | 16.65 |
| ATOM | 783 | C   | GLY | A | 118 | 6.186  | 18.761 | 26.901 | 1.00 | 15.21 |
| ATOM | 784 | O   | GLY | A | 118 | 6.087  | 19.352 | 27.989 | 1.00 | 16.22 |
| ATOM | 785 | N   | PRO | A | 119 | 6.035  | 17.445 | 26.822 | 1.00 | 15.88 |
| ATOM | 786 | CA  | PRO | A | 119 | 5.791  | 16.689 | 28.055 | 1.00 | 15.90 |
| ATOM | 787 | CB  | PRO | A | 119 | 5.878  | 15.243 | 27.582 | 1.00 | 17.35 |
| ATOM | 788 | CG  | PRO | A | 119 | 5.520  | 15.281 | 26.147 | 1.00 | 16.27 |
| ATOM | 789 | CD  | PRO | A | 119 | 6.092  | 16.575 | 25.628 | 1.00 | 16.39 |
| ATOM | 790 | C   | PRO | A | 119 | 6.768  | 16.949 | 29.213 | 1.00 | 17.04 |
| ATOM | 791 | O   | PRO | A | 119 | 7.972  | 17.127 | 28.997 | 1.00 | 17.25 |
| ATOM | 792 | N   | LEU | A | 120 | 6.230  | 16.986 | 30.427 | 1.00 | 20.34 |
| ATOM | 793 | CA  | LEU | A | 120 | 7.006  | 17.119 | 31.660 | 1.00 | 20.38 |
| ATOM | 794 | CB  | LEU | A | 120 | 6.171  | 17.875 | 32.683 | 1.00 | 20.80 |
| ATOM | 795 | CG  | LEU | A | 120 | 5.899  | 19.355 | 32.400 | 1.00 | 20.40 |
| ATOM | 796 | CD1 | LEU | A | 120 | 4.670  | 19.772 | 33.207 | 1.00 | 20.65 |
| ATOM | 797 | CD2 | LEU | A | 120 | 7.087  | 20.257 | 32.655 | 1.00 | 22.46 |
| ATOM | 798 | C   | LEU | A | 120 | 7.324  | 15.718 | 32.190 | 1.00 | 22.07 |
| ATOM | 799 | O   | LEU | A | 120 | 6.642  | 14.762 | 31.824 | 1.00 | 19.88 |
| ATOM | 800 | N   | PRO | A | 121 | 8.343  | 15.566 | 33.032 | 1.00 | 22.56 |
| ATOM | 801 | CA  | PRO | A | 121 | 8.590  | 14.265 | 33.676 | 1.00 | 22.53 |
| ATOM | 802 | CB  | PRO | A | 121 | 9.586  | 14.599 | 34.790 | 1.00 | 22.51 |
| ATOM | 803 | CG  | PRO | A | 121 | 10.302 | 15.799 | 34.270 | 1.00 | 24.46 |
| ATOM | 804 | CD  | PRO | A | 121 | 9.302  | 16.594 | 33.481 | 1.00 | 23.40 |
| ATOM | 805 | C   | PRO | A | 121 | 7.295  | 13.766 | 34.308 | 1.00 | 20.90 |
| ATOM | 806 | O   | PRO | A | 121 | 7.019  | 12.575 | 34.178 | 1.00 | 22.13 |
| ATOM | 807 | N   | GLY | A | 122 | 6.529  | 14.643 | 34.946 | 1.00 | 18.52 |
| ATOM | 808 | CA  | GLY | A | 122 | 5.267  | 14.247 | 35.555 | 1.00 | 19.71 |
| ATOM | 809 | C   | GLY | A | 122 | 4.050  | 14.113 | 34.658 | 1.00 | 19.48 |
| ATOM | 810 | O   | GLY | A | 122 | 3.008  | 13.713 | 35.158 | 1.00 | 20.10 |
| ATOM | 811 | N   | THR | A | 123 | 4.152  | 14.463 | 33.376 | 1.00 | 19.70 |
| ATOM | 812 | CA  | THR | A | 123 | 3.013  | 14.300 | 32.467 | 1.00 | 20.05 |
| ATOM | 813 | CB  | THR | A | 123 | 2.470  | 15.643 | 31.910 | 1.00 | 19.02 |
| ATOM | 814 | OG1 | THR | A | 123 | 3.417  | 16.229 | 31.006 | 1.00 | 17.75 |
| ATOM | 815 | CG2 | THR | A | 123 | 2.286  | 16.724 | 33.011 | 1.00 | 21.52 |
| ATOM | 816 | C   | THR | A | 123 | 3.305  | 13.389 | 31.279 | 1.00 | 18.26 |
| ATOM | 817 | O   | THR | A | 123 | 2.428  | 13.238 | 30.410 | 1.00 | 19.28 |
| ATOM | 818 | N   | LYS | A | 124 | 4.498  | 12.810 | 31.219 | 1.00 | 18.95 |
| ATOM | 819 | CA  | LYS | A | 124 | 4.788  | 11.956 | 30.057 | 1.00 | 18.96 |
| ATOM | 820 | CB  | LYS | A | 124 | 6.283  | 11.641 | 29.950 | 1.00 | 20.13 |
| ATOM | 821 | CG  | LYS | A | 124 | 6.834  | 10.806 | 31.086 | 1.00 | 23.04 |
| ATOM | 822 | CD  | LYS | A | 124 | 8.336  | 10.603 | 30.898 | 1.00 | 29.73 |
| ATOM | 823 | CE  | LYS | A | 124 | 8.775  | 9.445  | 31.787 | 1.00 | 36.02 |
| ATOM | 824 | NZ  | LYS | A | 124 | 10.152 | 9.706  | 32.286 | 1.00 | 43.04 |
| ATOM | 825 | C   | LYS | A | 124 | 3.876  | 10.734 | 29.956 | 1.00 | 19.08 |
| ATOM | 826 | O   | LYS | A | 124 | 3.538  | 10.312 | 28.855 | 1.00 | 17.17 |
| ATOM | 827 | N   | ASP | A | 125 | 3.454  | 10.156 | 31.086 | 1.00 | 18.94 |
| ATOM | 828 | CA  | ASP | A | 125 | 2.497  | 9.066  | 31.016 | 1.00 | 19.18 |
| ATOM | 829 | CB  | ASP | A | 125 | 2.272  | 8.426  | 32.390 | 1.00 | 20.53 |
| ATOM | 830 | CG  | ASP | A | 125 | 3.531  | 7.858  | 32.991 | 1.00 | 22.30 |
| ATOM | 831 | OD1 | ASP | A | 125 | 4.545  | 7.684  | 32.280 | 1.00 | 23.89 |

**FIGURE 268**



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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 832 | OD2 | ASP | A | 125 | 3.577  | 7.580  | 34.216 | 1.00 | 25.30 |
| ATOM | 833 | C   | ASP | A | 125 | 1.160  | 9.570  | 30.460 | 1.00 | 18.40 |
| ATOM | 834 | O   | ASP | A | 125 | 0.519  | 8.877  | 29.670 | 1.00 | 19.13 |
| ATOM | 835 | N   | ASP | A | 126 | 0.760  | 10.773 | 30.871 | 1.00 | 17.97 |
| ATOM | 836 | CA  | ASP | A | 126 | -0.453 | 11.402 | 30.351 | 1.00 | 17.81 |
| ATOM | 837 | CB  | ASP | A | 126 | -0.632 | 12.804 | 30.951 | 1.00 | 18.50 |
| ATOM | 838 | CG  | ASP | A | 126 | -0.832 | 12.813 | 32.447 | 1.00 | 24.65 |
| ATOM | 839 | OD1 | ASP | A | 126 | -1.196 | 11.774 | 33.046 | 1.00 | 22.46 |
| ATOM | 840 | OD2 | ASP | A | 126 | -0.670 | 13.887 | 33.085 | 1.00 | 24.22 |
| ATOM | 841 | C   | ASP | A | 126 | -0.314 | 11.606 | 28.837 | 1.00 | 16.85 |
| ATOM | 842 | O   | ASP | A | 126 | -1.256 | 11.407 | 28.082 | 1.00 | 16.48 |
| ATOM | 843 | N   | PHE | A | 127 | 0.868  | 12.008 | 28.380 | 1.00 | 17.92 |
| ATOM | 844 | CA  | PHE | A | 127 | 1.068  | 12.282 | 26.958 | 1.00 | 16.02 |
| ATOM | 845 | CB  | PHE | A | 127 | 2.459  | 12.901 | 26.744 | 1.00 | 15.67 |
| ATOM | 846 | CG  | PHE | A | 127 | 2.886  | 12.934 | 25.300 | 1.00 | 15.63 |
| ATOM | 847 | CD1 | PHE | A | 127 | 2.614  | 14.040 | 24.513 | 1.00 | 15.34 |
| ATOM | 848 | CE1 | PHE | A | 127 | 3.015  | 14.065 | 23.170 | 1.00 | 18.23 |
| ATOM | 849 | CZ  | PHE | A | 127 | 3.682  | 12.972 | 22.603 | 1.00 | 17.60 |
| ATOM | 850 | CE2 | PHE | A | 127 | 3.902  | 11.819 | 23.398 | 1.00 | 14.91 |
| ATOM | 851 | CD2 | PHE | A | 127 | 3.540  | 11.826 | 24.721 | 1.00 | 15.74 |
| ATOM | 852 | C   | PHE | A | 127 | 0.913  | 10.967 | 26.199 | 1.00 | 15.37 |
| ATOM | 853 | O   | PHE | A | 127 | 0.234  | 10.922 | 25.167 | 1.00 | 15.38 |
| ATOM | 854 | N   | TRP | A | 128 | 1.486  | 9.880  | 26.710 | 1.00 | 15.77 |
| ATOM | 855 | CA  | TRP | A | 128 | 1.412  | 8.643  | 25.951 | 1.00 | 15.30 |
| ATOM | 856 | CB  | TRP | A | 128 | 2.416  | 7.618  | 26.452 | 1.00 | 14.62 |
| ATOM | 857 | CG  | TRP | A | 128 | 3.800  | 7.961  | 26.004 | 1.00 | 15.64 |
| ATOM | 858 | CD1 | TRP | A | 128 | 4.848  | 8.266  | 26.796 | 1.00 | 16.32 |
| ATOM | 859 | NE1 | TRP | A | 128 | 5.978  | 8.498  | 26.047 | 1.00 | 16.04 |
| ATOM | 860 | CE2 | TRP | A | 128 | 5.658  | 8.340  | 24.721 | 1.00 | 17.00 |
| ATOM | 861 | CD2 | TRP | A | 128 | 4.275  | 8.037  | 24.656 | 1.00 | 14.14 |
| ATOM | 862 | CE3 | TRP | A | 128 | 3.697  | 7.798  | 23.401 | 1.00 | 18.83 |
| ATOM | 863 | CZ3 | TRP | A | 128 | 4.481  | 7.947  | 22.261 | 1.00 | 19.71 |
| ATOM | 864 | CH2 | TRP | A | 128 | 5.855  | 8.288  | 22.362 | 1.00 | 18.66 |
| ATOM | 865 | CZ2 | TRP | A | 128 | 6.446  | 8.494  | 23.583 | 1.00 | 17.54 |
| ATOM | 866 | C   | TRP | A | 128 | 0.000  | 8.071  | 25.981 | 1.00 | 14.42 |
| ATOM | 867 | O   | TRP | A | 128 | -0.410 | 7.416  | 25.021 | 1.00 | 15.80 |
| ATOM | 868 | N   | LYS | A | 129 | -0.671 | 8.219  | 27.123 | 1.00 | 16.32 |
| ATOM | 869 | CA  | LYS | A | 129 | -2.091 | 7.905  | 27.214 | 1.00 | 15.35 |
| ATOM | 870 | CB  | LYS | A | 129 | -2.642 | 8.310  | 28.588 | 1.00 | 18.04 |
| ATOM | 871 | CG  | LYS | A | 129 | -4.131 | 7.953  | 28.762 | 1.00 | 16.84 |
| ATOM | 872 | CD  | LYS | A | 129 | -4.549 | 8.066  | 30.229 | 1.00 | 19.80 |
| ATOM | 873 | CE  | LYS | A | 129 | -6.064 | 8.051  | 30.343 | 1.00 | 21.91 |
| ATOM | 874 | NZ  | LYS | A | 129 | -6.439 | 8.260  | 31.807 | 1.00 | 25.23 |
| ATOM | 875 | C   | LYS | A | 129 | -2.861 | 8.607  | 26.121 | 1.00 | 16.69 |
| ATOM | 876 | O   | LYS | A | 129 | -3.713 | 8.011  | 25.465 | 1.00 | 16.75 |
| ATOM | 877 | N   | MET | A | 130 | -2.618 | 9.909  | 25.990 | 1.00 | 15.72 |
| ATOM | 878 | CA  | MET | A | 130 | -3.311 | 10.652 | 24.957 | 1.00 | 16.87 |
| ATOM | 879 | CB  | MET | A | 130 | -3.026 | 12.145 | 25.080 | 1.00 | 14.45 |
| ATOM | 880 | CG  | MET | A | 130 | -3.608 | 12.865 | 23.908 | 1.00 | 15.57 |
| ATOM | 881 | SD  | MET | A | 130 | -3.131 | 14.614 | 23.936 | 1.00 | 17.91 |
| ATOM | 882 | CE  | MET | A | 130 | -1.383 | 14.608 | 23.583 | 1.00 | 16.03 |
| ATOM | 883 | C   | MET | A | 130 | -3.040 | 10.117 | 23.548 | 1.00 | 16.34 |

**FIGURE 269**

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Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 884 | O   | MET | A | 130 | -3.965 | 9.899  | 22.759 | 1.00 | 16.31 |
| ATOM | 885 | N   | VAL | A | 131 | -1.783 | 9.837  | 23.226 | 1.00 | 15.65 |
| ATOM | 886 | CA  | VAL | A | 131 | -1.402 | 9.283  | 21.924 | 1.00 | 13.92 |
| ATOM | 887 | CB  | VAL | A | 131 | 0.120  | 9.049  | 21.956 | 1.00 | 14.34 |
| ATOM | 888 | CG1 | VAL | A | 131 | 0.588  | 8.212  | 20.797 | 1.00 | 18.45 |
| ATOM | 889 | CG2 | VAL | A | 131 | 0.877  | 10.386 | 21.984 | 1.00 | 18.04 |
| ATOM | 890 | C   | VAL | A | 131 | -2.107 | 7.948  | 21.681 | 1.00 | 14.86 |
| ATOM | 891 | O   | VAL | A | 131 | -2.609 | 7.668  | 20.579 | 1.00 | 15.81 |
| ATOM | 892 | N   | TRP | A | 132 | -2.209 | 7.145  | 22.732 | 1.00 | 14.88 |
| ATOM | 893 | CA  | TRP | A | 132 | -2.840 | 5.840  | 22.599 | 1.00 | 14.40 |
| ATOM | 894 | CB  | TRP | A | 132 | -2.599 | 4.996  | 23.861 | 1.00 | 14.68 |
| ATOM | 895 | CG  | TRP | A | 132 | -3.301 | 3.666  | 23.747 | 1.00 | 16.82 |
| ATOM | 896 | CD1 | TRP | A | 132 | -4.427 | 3.273  | 24.402 | 1.00 | 17.83 |
| ATOM | 897 | NE1 | TRP | A | 132 | -4.799 | 2.015  | 23.980 | 1.00 | 16.10 |
| ATOM | 898 | CE2 | TRP | A | 132 | -3.901 | 1.566  | 23.049 | 1.00 | 19.18 |
| ATOM | 899 | CD2 | TRP | A | 132 | -2.956 | 2.591  | 22.852 | 1.00 | 18.23 |
| ATOM | 900 | CE3 | TRP | A | 132 | -1.924 | 2.388  | 21.930 | 1.00 | 16.64 |
| ATOM | 901 | CZ3 | TRP | A | 132 | -1.857 | 1.165  | 21.233 | 1.00 | 18.77 |
| ATOM | 902 | CH2 | TRP | A | 132 | -2.841 | 0.177  | 21.450 | 1.00 | 19.47 |
| ATOM | 903 | CZ2 | TRP | A | 132 | -3.857 | 0.358  | 22.350 | 1.00 | 18.87 |
| ATOM | 904 | C   | TRP | A | 132 | -4.346 | 6.021  | 22.375 | 1.00 | 14.57 |
| ATOM | 905 | O   | TRP | A | 132 | -4.901 | 5.489  | 21.423 | 1.00 | 14.81 |
| ATOM | 906 | N   | GLU | A | 133 | -4.977 | 6.784  | 23.257 | 1.00 | 17.42 |
| ATOM | 907 | CA  | GLU | A | 133 | -6.450 | 6.895  | 23.277 | 1.00 | 15.50 |
| ATOM | 908 | CB  | GLU | A | 133 | -6.924 | 7.614  | 24.526 | 1.00 | 15.78 |
| ATOM | 909 | CG  | GLU | A | 133 | -6.669 | 6.814  | 25.790 | 1.00 | 17.18 |
| ATOM | 910 | CD  | GLU | A | 133 | -7.390 | 7.374  | 26.988 | 1.00 | 25.51 |
| ATOM | 911 | OE1 | GLU | A | 133 | -7.721 | 8.585  | 26.977 | 1.00 | 22.92 |
| ATOM | 912 | OE2 | GLU | A | 133 | -7.539 | 6.592  | 27.957 | 1.00 | 21.86 |
| ATOM | 913 | C   | GLU | A | 133 | -6.990 | 7.595  | 22.041 | 1.00 | 17.24 |
| ATOM | 914 | O   | GLU | A | 133 | -8.144 | 7.335  | 21.609 | 1.00 | 16.93 |
| ATOM | 915 | N   | GLN | A | 134 | -6.188 | 8.513  | 21.501 | 1.00 | 16.12 |
| ATOM | 916 | CA  | GLN | A | 134 | -6.583 | 9.284  | 20.326 | 1.00 | 16.01 |
| ATOM | 917 | CB  | GLN | A | 134 | -6.136 | 10.746 | 20.432 | 1.00 | 15.45 |
| ATOM | 918 | CG  | GLN | A | 134 | -6.658 | 11.461 | 21.657 | 1.00 | 16.97 |
| ATOM | 919 | CD  | GLN | A | 134 | -8.141 | 11.671 | 21.576 | 1.00 | 21.63 |
| ATOM | 920 | OE1 | GLN | A | 134 | -8.649 | 12.128 | 20.548 | 1.00 | 30.42 |
| ATOM | 921 | NE2 | GLN | A | 134 | -8.855 | 11.298 | 22.636 | 1.00 | 24.38 |
| ATOM | 922 | C   | GLN | A | 134 | -6.211 | 8.681  | 18.987 | 1.00 | 16.29 |
| ATOM | 923 | O   | GLN | A | 134 | -6.418 | 9.300  | 17.936 | 1.00 | 17.57 |
| ATOM | 924 | N   | ASN | A | 135 | -5.721 | 7.438  | 19.007 | 1.00 | 16.26 |
| ATOM | 925 | CA  | ASN | A | 135 | -5.338 | 6.741  | 17.788 | 1.00 | 16.42 |
| ATOM | 926 | CB  | ASN | A | 135 | -6.562 | 6.516  | 16.901 | 1.00 | 18.03 |
| ATOM | 927 | CG  | ASN | A | 135 | -7.602 | 5.656  | 17.580 | 1.00 | 22.43 |
| ATOM | 928 | OD1 | ASN | A | 135 | -7.358 | 4.475  | 17.849 | 1.00 | 28.78 |
| ATOM | 929 | ND2 | ASN | A | 135 | -8.757 | 6.232  | 17.865 | 1.00 | 27.37 |
| ATOM | 930 | C   | ASN | A | 135 | -4.243 | 7.426  | 16.964 | 1.00 | 18.21 |
| ATOM | 931 | O   | ASN | A | 135 | -4.199 | 7.287  | 15.749 | 1.00 | 17.34 |
| ATOM | 932 | N   | VAL | A | 136 | -3.380 | 8.164  | 17.651 | 1.00 | 18.13 |
| ATOM | 933 | CA  | VAL | A | 136 | -2.276 | 8.873  | 17.011 | 1.00 | 16.80 |
| ATOM | 934 | CB  | VAL | A | 136 | -1.664 | 9.866  | 18.023 | 1.00 | 18.00 |
| ATOM | 935 | CG1 | VAL | A | 136 | -0.351 | 10.461 | 17.482 | 1.00 | 16.01 |

**FIGURE 270**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |     |     |     |   |     |        |        |        |      |       |
|------|-----|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 936 | CG2 | VAL | A | 136 | -2.680 | 10.930 | 18.399 | 1.00 | 18.19 |
| ATOM | 937 | C   | VAL | A | 136 | -1.229 | 7.880  | 16.483 | 1.00 | 18.93 |
| ATOM | 938 | O   | VAL | A | 136 | -0.821 | 6.977  | 17.211 | 1.00 | 19.57 |
| ATOM | 939 | N   | HIS | A | 137 | -0.860 | 8.013  | 15.202 | 1.00 | 17.50 |
| ATOM | 940 | CA  | HIS | A | 137 | 0.264  | 7.277  | 14.623 | 1.00 | 16.22 |
| ATOM | 941 | CB  | HIS | A | 137 | -0.110 | 6.473  | 13.360 | 1.00 | 18.79 |
| ATOM | 942 | CG  | HIS | A | 137 | -1.152 | 5.414  | 13.571 | 1.00 | 19.38 |
| ATOM | 943 | ND1 | HIS | A | 137 | -2.419 | 5.691  | 14.034 | 1.00 | 20.18 |
| ATOM | 944 | CE1 | HIS | A | 137 | -3.116 | 4.572  | 14.115 | 1.00 | 22.60 |
| ATOM | 945 | NE2 | HIS | A | 137 | -2.358 | 3.579  | 13.680 | 1.00 | 22.19 |
| ATOM | 946 | CD2 | HIS | A | 137 | -1.121 | 4.078  | 13.344 | 1.00 | 20.32 |
| ATOM | 947 | C   | HIS | A | 137 | 1.494  | 8.093  | 14.295 | 1.00 | 17.23 |
| ATOM | 948 | O   | HIS | A | 137 | 2.513  | 7.496  | 13.947 | 1.00 | 17.71 |
| ATOM | 949 | N   | ASN | A | 138 | 1.428  | 9.423  | 14.394 | 1.00 | 16.24 |
| ATOM | 950 | CA  | ASN | A | 138 | 2.590  | 10.238 | 14.046 | 1.00 | 17.25 |
| ATOM | 951 | CB  | ASN | A | 138 | 2.470  | 10.816 | 12.632 | 1.00 | 17.99 |
| ATOM | 952 | CG  | ASN | A | 138 | 2.330  | 9.741  | 11.562 | 1.00 | 18.27 |
| ATOM | 953 | OD1 | ASN | A | 138 | 1.219  | 9.397  | 11.126 | 1.00 | 25.07 |
| ATOM | 954 | ND2 | ASN | A | 138 | 3.457  | 9.169  | 11.189 | 1.00 | 19.74 |
| ATOM | 955 | C   | ASN | A | 138 | 2.684  | 11.382 | 15.044 | 1.00 | 14.09 |
| ATOM | 956 | O   | ASN | A | 138 | 1.676  | 11.996 | 15.397 | 1.00 | 15.42 |
| ATOM | 957 | N   | ILE | A | 139 | 3.904  | 11.633 | 15.485 | 1.00 | 13.67 |
| ATOM | 958 | CA  | ILE | A | 139 | 4.204  | 12.739 | 16.391 | 1.00 | 13.12 |
| ATOM | 959 | CB  | ILE | A | 139 | 4.750  | 12.186 | 17.716 | 1.00 | 14.52 |
| ATOM | 960 | CG1 | ILE | A | 139 | 3.714  | 11.302 | 18.394 | 1.00 | 14.31 |
| ATOM | 961 | CD1 | ILE | A | 139 | 4.274  | 10.494 | 19.577 | 1.00 | 15.81 |
| ATOM | 962 | CG2 | ILE | A | 139 | 5.125  | 13.346 | 18.653 | 1.00 | 15.50 |
| ATOM | 963 | C   | ILE | A | 139 | 5.282  | 13.581 | 15.752 | 1.00 | 15.31 |
| ATOM | 964 | O   | ILE | A | 139 | 6.323  | 13.073 | 15.333 | 1.00 | 16.48 |
| ATOM | 965 | N   | VAL | A | 140 | 5.076  | 14.892 | 15.788 | 1.00 | 14.75 |
| ATOM | 966 | CA  | VAL | A | 140 | 6.049  | 15.831 | 15.231 | 1.00 | 15.93 |
| ATOM | 967 | CB  | VAL | A | 140 | 5.367  | 16.704 | 14.177 | 1.00 | 15.43 |
| ATOM | 968 | CG1 | VAL | A | 140 | 6.329  | 17.788 | 13.728 | 1.00 | 16.73 |
| ATOM | 969 | CG2 | VAL | A | 140 | 4.898  | 15.852 | 12.985 | 1.00 | 17.63 |
| ATOM | 970 | C   | VAL | A | 140 | 6.531  | 16.700 | 16.377 | 1.00 | 16.09 |
| ATOM | 971 | O   | VAL | A | 140 | 5.717  | 17.295 | 17.053 | 1.00 | 18.31 |
| ATOM | 972 | N   | MET | A | 141 | 7.839  | 16.702 | 16.645 | 1.00 | 16.31 |
| ATOM | 973 | CA  | MET | A | 141 | 8.421  | 17.472 | 17.741 | 1.00 | 17.39 |
| ATOM | 974 | CB  | MET | A | 141 | 9.226  | 16.515 | 18.632 | 1.00 | 16.11 |
| ATOM | 975 | CG  | MET | A | 141 | 10.082 | 17.201 | 19.670 | 1.00 | 16.87 |
| ATOM | 976 | SD  | MET | A | 141 | 10.679 | 15.960 | 20.837 | 1.00 | 18.61 |
| ATOM | 977 | CE  | MET | A | 141 | 11.650 | 16.998 | 21.959 | 1.00 | 19.51 |
| ATOM | 978 | C   | MET | A | 141 | 9.344  | 18.530 | 17.127 | 1.00 | 17.17 |
| ATOM | 979 | O   | MET | A | 141 | 10.303 | 18.177 | 16.439 | 1.00 | 17.62 |
| ATOM | 980 | N   | VAL | A | 142 | 9.081  | 19.805 | 17.364 | 1.00 | 16.69 |
| ATOM | 981 | CA  | VAL | A | 142 | 9.869  | 20.876 | 16.731 | 1.00 | 19.57 |
| ATOM | 982 | CB  | VAL | A | 142 | 9.050  | 21.674 | 15.715 | 1.00 | 17.61 |
| ATOM | 983 | CG1 | VAL | A | 142 | 8.808  | 20.820 | 14.463 | 1.00 | 20.20 |
| ATOM | 984 | CG2 | VAL | A | 142 | 7.675  | 22.009 | 16.283 | 1.00 | 19.28 |
| ATOM | 985 | C   | VAL | A | 142 | 10.477 | 21.756 | 17.829 | 1.00 | 21.83 |
| ATOM | 986 | O   | VAL | A | 142 | 10.473 | 22.986 | 17.763 | 1.00 | 24.11 |
| ATOM | 987 | N   | THR | A | 143 | 10.993 | 21.091 | 18.852 | 1.00 | 19.91 |

**FIGURE 271**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 988  | CA  | THR | A | 143 | 11.845 | 21.727 | 19.857 | 1.00 | 20.81 |
| ATOM | 989  | CB  | THR | A | 143 | 11.042 | 22.039 | 21.108 | 1.00 | 20.61 |
| ATOM | 990  | OG1 | THR | A | 143 | 11.835 | 22.818 | 22.014 | 1.00 | 20.47 |
| ATOM | 991  | CG2 | THR | A | 143 | 10.728 | 20.749 | 21.898 | 1.00 | 19.53 |
| ATOM | 992  | C   | THR | A | 143 | 13.001 | 20.795 | 20.195 | 1.00 | 21.41 |
| ATOM | 993  | O   | THR | A | 143 | 12.919 | 19.603 | 19.953 | 1.00 | 20.95 |
| ATOM | 994  | N   | GLN | A | 144 | 14.096 | 21.337 | 20.719 | 1.00 | 21.06 |
| ATOM | 995  | CA  | GLN | A | 144 | 15.047 | 20.523 | 21.456 | 1.00 | 21.41 |
| ATOM | 996  | CB  | GLN | A | 144 | 16.453 | 21.107 | 21.274 | 1.00 | 20.22 |
| ATOM | 997  | CG  | GLN | A | 144 | 16.883 | 21.003 | 19.815 | 1.00 | 24.39 |
| ATOM | 998  | CD  | GLN | A | 144 | 18.359 | 21.298 | 19.583 | 1.00 | 35.02 |
| ATOM | 999  | OE1 | GLN | A | 144 | 19.223 | 20.456 | 19.834 | 1.00 | 39.33 |
| ATOM | 1000 | NE2 | GLN | A | 144 | 18.645 | 22.494 | 19.082 | 1.00 | 39.04 |
| ATOM | 1001 | C   | GLN | A | 144 | 14.654 | 20.440 | 22.930 | 1.00 | 21.42 |
| ATOM | 1002 | O   | GLN | A | 144 | 13.847 | 21.248 | 23.418 | 1.00 | 22.29 |
| ATOM | 1003 | N   | CYS | A | 145 | 15.180 | 19.442 | 23.633 | 1.00 | 22.65 |
| ATOM | 1004 | CA  | CYS | A | 145 | 14.894 | 19.289 | 25.055 | 1.00 | 21.56 |
| ATOM | 1005 | CB  | CYS | A | 145 | 15.328 | 17.917 | 25.563 | 1.00 | 24.41 |
| ATOM | 1006 | SG  | CYS | A | 145 | 14.340 | 16.594 | 24.859 | 1.00 | 25.88 |
| ATOM | 1007 | C   | CYS | A | 145 | 15.512 | 20.364 | 25.934 | 1.00 | 22.77 |
| ATOM | 1008 | O   | CYS | A | 145 | 14.891 | 20.755 | 26.915 | 1.00 | 24.26 |
| ATOM | 1009 | N   | VAL | A | 146 | 16.719 | 20.828 | 25.592 | 1.00 | 23.87 |
| ATOM | 1010 | CA  | VAL | A | 146 | 17.339 | 21.968 | 26.261 | 1.00 | 23.79 |
| ATOM | 1011 | CB  | VAL | A | 146 | 18.563 | 21.575 | 27.130 | 1.00 | 24.52 |
| ATOM | 1012 | CG1 | VAL | A | 146 | 19.148 | 22.814 | 27.803 | 1.00 | 25.21 |
| ATOM | 1013 | CG2 | VAL | A | 146 | 18.189 | 20.488 | 28.141 | 1.00 | 23.81 |
| ATOM | 1014 | C   | VAL | A | 146 | 17.767 | 22.977 | 25.204 | 1.00 | 24.71 |
| ATOM | 1015 | O   | VAL | A | 146 | 18.313 | 22.613 | 24.157 | 1.00 | 25.61 |
| ATOM | 1016 | N   | GLU | A | 147 | 17.443 | 24.238 | 25.459 | 1.00 | 25.28 |
| ATOM | 1017 | CA  | GLU | A | 147 | 17.691 | 25.313 | 24.508 | 1.00 | 27.56 |
| ATOM | 1018 | CB  | GLU | A | 147 | 16.406 | 25.661 | 23.747 | 1.00 | 26.39 |
| ATOM | 1019 | CG  | GLU | A | 147 | 16.147 | 24.689 | 22.609 | 1.00 | 27.32 |
| ATOM | 1020 | CD  | GLU | A | 147 | 14.780 | 24.858 | 21.965 | 1.00 | 30.78 |
| ATOM | 1021 | OE1 | GLU | A | 147 | 13.981 | 25.680 | 22.460 | 1.00 | 34.57 |
| ATOM | 1022 | OE2 | GLU | A | 147 | 14.494 | 24.143 | 20.984 | 1.00 | 29.08 |
| ATOM | 1023 | C   | GLU | A | 147 | 18.200 | 26.521 | 25.286 | 1.00 | 29.05 |
| ATOM | 1024 | O   | GLU | A | 147 | 17.526 | 27.046 | 26.173 | 1.00 | 29.89 |
| ATOM | 1025 | N   | LYS | A | 148 | 19.419 | 26.935 | 24.961 | 1.00 | 32.08 |
| ATOM | 1026 | CA  | LYS | A | 148 | 20.039 | 28.057 | 25.662 | 1.00 | 33.87 |
| ATOM | 1027 | CB  | LYS | A | 148 | 19.459 | 29.383 | 25.157 | 1.00 | 34.11 |
| ATOM | 1028 | CG  | LYS | A | 148 | 19.601 | 29.554 | 23.639 | 1.00 | 39.02 |
| ATOM | 1029 | CD  | LYS | A | 148 | 19.140 | 30.923 | 23.161 | 1.00 | 46.18 |
| ATOM | 1030 | CE  | LYS | A | 148 | 19.201 | 31.029 | 21.638 | 1.00 | 46.64 |
| ATOM | 1031 | NZ  | LYS | A | 148 | 18.688 | 32.332 | 21.111 | 1.00 | 48.93 |
| ATOM | 1032 | C   | LYS | A | 148 | 19.970 | 27.934 | 27.190 | 1.00 | 32.87 |
| ATOM | 1033 | O   | LYS | A | 148 | 19.718 | 28.910 | 27.909 | 1.00 | 34.86 |
| ATOM | 1034 | N   | GLY | A | 149 | 20.203 | 26.721 | 27.676 | 1.00 | 32.51 |
| ATOM | 1035 | CA  | GLY | A | 149 | 20.364 | 26.475 | 29.100 | 1.00 | 31.75 |
| ATOM | 1036 | C   | GLY | A | 149 | 19.065 | 26.281 | 29.850 | 1.00 | 32.98 |
| ATOM | 1037 | O   | GLY | A | 149 | 19.060 | 26.224 | 31.078 | 1.00 | 34.77 |
| ATOM | 1038 | N   | ARG | A | 150 | 17.960 | 26.198 | 29.113 | 1.00 | 28.60 |
| ATOM | 1039 | CA  | ARG | A | 150 | 16.636 | 26.155 | 29.727 | 1.00 | 29.87 |

**FIGURE 272**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1040 | CB  | ARG | A | 150 | 15.753 | 27.256 | 29.140 | 1.00 | 27.76 |
| ATOM | 1041 | CG  | ARG | A | 150 | 14.682 | 27.764 | 30.090 | 1.00 | 38.86 |
| ATOM | 1042 | CD  | ARG | A | 150 | 13.434 | 26.895 | 30.207 | 1.00 | 47.60 |
| ATOM | 1043 | NE  | ARG | A | 150 | 12.793 | 27.055 | 31.514 | 1.00 | 53.99 |
| ATOM | 1044 | CZ  | ARG | A | 150 | 11.684 | 27.754 | 31.725 | 1.00 | 57.80 |
| ATOM | 1045 | NH1 | ARG | A | 150 | 11.080 | 28.354 | 30.708 | 1.00 | 60.31 |
| ATOM | 1046 | NH2 | ARG | A | 150 | 11.170 | 27.851 | 32.947 | 1.00 | 59.21 |
| ATOM | 1047 | C   | ARG | A | 150 | 16.059 | 24.827 | 29.300 | 1.00 | 26.37 |
| ATOM | 1048 | O   | ARG | A | 150 | 16.204 | 24.456 | 28.136 | 1.00 | 26.29 |
| ATOM | 1049 | N   | VAL | A | 151 | 15.407 | 24.129 | 30.226 | 1.00 | 27.16 |
| ATOM | 1050 | CA  | VAL | A | 151 | 14.784 | 22.862 | 29.876 | 1.00 | 26.73 |
| ATOM | 1051 | CB  | VAL | A | 151 | 14.567 | 21.979 | 31.132 | 1.00 | 27.55 |
| ATOM | 1052 | CG1 | VAL | A | 151 | 13.608 | 20.849 | 30.835 | 1.00 | 25.30 |
| ATOM | 1053 | CG2 | VAL | A | 151 | 15.909 | 21.399 | 31.605 | 1.00 | 29.25 |
| ATOM | 1054 | C   | VAL | A | 151 | 13.486 | 23.199 | 29.136 | 1.00 | 24.76 |
| ATOM | 1055 | O   | VAL | A | 151 | 12.697 | 24.027 | 29.612 | 1.00 | 28.00 |
| ATOM | 1056 | N   | LYS | A | 152 | 13.285 | 22.595 | 27.964 | 1.00 | 23.05 |
| ATOM | 1057 | CA  | LYS | A | 152 | 12.147 | 22.954 | 27.114 | 1.00 | 23.12 |
| ATOM | 1058 | CB  | LYS | A | 152 | 12.622 | 23.481 | 25.741 | 1.00 | 24.16 |
| ATOM | 1059 | CG  | LYS | A | 152 | 13.479 | 24.753 | 25.812 | 1.00 | 26.71 |
| ATOM | 1060 | CD  | LYS | A | 152 | 12.677 | 26.053 | 25.966 | 1.00 | 31.53 |
| ATOM | 1061 | CE  | LYS | A | 152 | 13.274 | 27.189 | 25.109 | 1.00 | 31.75 |
| ATOM | 1062 | NZ  | LYS | A | 152 | 13.081 | 28.512 | 25.766 | 1.00 | 39.48 |
| ATOM | 1063 | C   | LYS | A | 152 | 11.170 | 21.809 | 26.923 | 1.00 | 22.29 |
| ATOM | 1064 | O   | LYS | A | 152 | 9.987  | 22.029 | 26.641 | 1.00 | 18.68 |
| ATOM | 1065 | N   | CYS | A | 153 | 11.677 | 20.599 | 27.139 | 1.00 | 22.37 |
| ATOM | 1066 | CA  | CYS | A | 153 | 10.914 | 19.385 | 26.901 | 1.00 | 20.12 |
| ATOM | 1067 | CB  | CYS | A | 153 | 10.752 | 19.107 | 25.412 | 1.00 | 19.37 |
| ATOM | 1068 | SG  | CYS | A | 153 | 9.611  | 17.737 | 25.063 | 1.00 | 18.76 |
| ATOM | 1069 | C   | CYS | A | 153 | 11.640 | 18.241 | 27.567 | 1.00 | 20.48 |
| ATOM | 1070 | O   | CYS | A | 153 | 12.868 | 18.148 | 27.498 | 1.00 | 21.39 |
| ATOM | 1071 | N   | ASP | A | 154 | 10.892 | 17.375 | 28.230 | 1.00 | 21.01 |
| ATOM | 1072 | CA  | ASP | A | 154 | 11.490 | 16.164 | 28.782 | 1.00 | 20.95 |
| ATOM | 1073 | CB  | ASP | A | 154 | 10.524 | 15.523 | 29.772 | 1.00 | 21.87 |
| ATOM | 1074 | CG  | ASP | A | 154 | 11.150 | 14.365 | 30.511 | 1.00 | 25.17 |
| ATOM | 1075 | OD1 | ASP | A | 154 | 12.202 | 14.589 | 31.155 | 1.00 | 24.97 |
| ATOM | 1076 | OD2 | ASP | A | 154 | 10.662 | 13.223 | 30.477 | 1.00 | 24.65 |
| ATOM | 1077 | C   | ASP | A | 154 | 11.831 | 15.185 | 27.650 | 1.00 | 20.85 |
| ATOM | 1078 | O   | ASP | A | 154 | 11.233 | 15.218 | 26.586 | 1.00 | 20.84 |
| ATOM | 1079 | N   | HIS | A | 155 | 12.838 | 14.337 | 27.860 | 1.00 | 20.25 |
| ATOM | 1080 | CA  | HIS | A | 155 | 13.113 | 13.265 | 26.916 | 1.00 | 20.35 |
| ATOM | 1081 | CB  | HIS | A | 155 | 14.579 | 12.839 | 27.069 | 1.00 | 21.06 |
| ATOM | 1082 | CG  | HIS | A | 155 | 15.056 | 11.901 | 26.007 | 1.00 | 22.85 |
| ATOM | 1083 | ND1 | HIS | A | 155 | 14.630 | 10.591 | 25.915 | 1.00 | 25.15 |
| ATOM | 1084 | CE1 | HIS | A | 155 | 15.237 | 10.003 | 24.900 | 1.00 | 24.10 |
| ATOM | 1085 | NE2 | HIS | A | 155 | 16.056 | 10.877 | 24.340 | 1.00 | 27.20 |
| ATOM | 1086 | CD2 | HIS | A | 155 | 15.975 | 12.067 | 25.026 | 1.00 | 27.39 |
| ATOM | 1087 | C   | HIS | A | 155 | 12.157 | 12.112 | 27.240 | 1.00 | 20.30 |
| ATOM | 1088 | O   | HIS | A | 155 | 12.458 | 11.225 | 28.053 | 1.00 | 19.64 |
| ATOM | 1089 | N   | TYR | A | 156 | 10.960 | 12.181 | 26.666 | 1.00 | 19.16 |
| ATOM | 1090 | CA  | TYR | A | 156 | 9.814  | 11.436 | 27.165 | 1.00 | 18.36 |
| ATOM | 1091 | CB  | TYR | A | 156 | 8.520  | 12.247 | 27.004 | 1.00 | 18.65 |

FIGURE 273

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1092 | CG  | TYR | A | 156 | 8.250  | 12.664 | 25.569 | 1.00 | 17.99 |
| ATOM | 1093 | CD1 | TYR | A | 156 | 7.624  | 11.796 | 24.669 | 1.00 | 16.25 |
| ATOM | 1094 | CE1 | TYR | A | 156 | 7.427  | 12.171 | 23.328 | 1.00 | 16.10 |
| ATOM | 1095 | CZ  | TYR | A | 156 | 7.776  | 13.457 | 22.936 | 1.00 | 15.17 |
| ATOM | 1096 | OH  | TYR | A | 156 | 7.497  | 13.806 | 21.627 | 1.00 | 15.03 |
| ATOM | 1097 | CE2 | TYR | A | 156 | 8.397  | 14.321 | 23.810 | 1.00 | 21.32 |
| ATOM | 1098 | CD2 | TYR | A | 156 | 8.618  | 13.922 | 25.132 | 1.00 | 16.85 |
| ATOM | 1099 | C   | TYR | A | 156 | 9.678  | 10.091 | 26.469 | 1.00 | 17.96 |
| ATOM | 1100 | O   | TYR | A | 156 | 8.723  | 9.365  | 26.730 | 1.00 | 18.06 |
| ATOM | 1101 | N   | TRP | A | 157 | 10.660 | 9.764  | 25.635 | 1.00 | 19.28 |
| ATOM | 1102 | CA  | TRP | A | 157 | 10.722 | 8.482  | 24.933 | 1.00 | 20.13 |
| ATOM | 1103 | CB  | TRP | A | 157 | 10.668 | 8.723  | 23.414 | 1.00 | 18.70 |
| ATOM | 1104 | CG  | TRP | A | 157 | 11.885 | 9.431  | 22.911 | 1.00 | 18.38 |
| ATOM | 1105 | CD1 | TRP | A | 157 | 13.031 | 8.858  | 22.463 | 1.00 | 20.53 |
| ATOM | 1106 | NE1 | TRP | A | 157 | 13.924 | 9.827  | 22.075 | 1.00 | 19.49 |
| ATOM | 1107 | CE2 | TRP | A | 157 | 13.387 | 11.061 | 22.338 | 1.00 | 17.77 |
| ATOM | 1108 | CD2 | TRP | A | 157 | 12.085 | 10.848 | 22.833 | 1.00 | 18.54 |
| ATOM | 1109 | CE3 | TRP | A | 157 | 11.320 | 11.955 | 23.192 | 1.00 | 20.35 |
| ATOM | 1110 | CZ3 | TRP | A | 157 | 11.836 | 13.222 | 23.012 | 1.00 | 20.87 |
| ATOM | 1111 | CH2 | TRP | A | 157 | 13.145 | 13.404 | 22.500 | 1.00 | 22.03 |
| ATOM | 1112 | CZ2 | TRP | A | 157 | 13.920 | 12.335 | 22.150 | 1.00 | 20.41 |
| ATOM | 1113 | C   | TRP | A | 157 | 11.993 | 7.755  | 25.370 | 1.00 | 22.07 |
| ATOM | 1114 | O   | TRP | A | 157 | 12.912 | 8.357  | 25.928 | 1.00 | 21.87 |
| ATOM | 1115 | N   | PRO | A | 158 | 12.042 | 6.446  | 25.173 | 1.00 | 23.81 |
| ATOM | 1116 | CA  | PRO | A | 158 | 13.207 | 5.671  | 25.615 | 1.00 | 25.18 |
| ATOM | 1117 | CB  | PRO | A | 158 | 12.854 | 4.227  | 25.238 | 1.00 | 25.31 |
| ATOM | 1118 | CG  | PRO | A | 158 | 11.341 | 4.234  | 25.220 | 1.00 | 24.87 |
| ATOM | 1119 | CD  | PRO | A | 158 | 10.976 | 5.594  | 24.619 | 1.00 | 25.87 |
| ATOM | 1120 | C   | PRO | A | 158 | 14.515 | 6.105  | 24.973 | 1.00 | 24.62 |
| ATOM | 1121 | O   | PRO | A | 158 | 14.568 | 6.599  | 23.836 | 1.00 | 24.33 |
| ATOM | 1122 | N   | ALA | A | 159 | 15.567 | 5.872  | 25.742 | 1.00 | 25.95 |
| ATOM | 1123 | CA  | ALA | A | 159 | 16.937 | 6.192  | 25.347 | 1.00 | 27.03 |
| ATOM | 1124 | CB  | ALA | A | 159 | 17.775 | 6.378  | 26.592 | 1.00 | 26.95 |
| ATOM | 1125 | C   | ALA | A | 159 | 17.529 | 5.113  | 24.441 | 1.00 | 28.60 |
| ATOM | 1126 | O   | ALA | A | 159 | 18.512 | 5.345  | 23.723 | 1.00 | 31.08 |
| ATOM | 1127 | N   | ASP | A | 160 | 16.921 | 3.932  | 24.461 | 1.00 | 26.27 |
| ATOM | 1128 | CA  | ASP | A | 160 | 17.429 | 2.795  | 23.710 | 1.00 | 26.44 |
| ATOM | 1129 | CB  | ASP | A | 160 | 18.488 | 2.056  | 24.529 | 1.00 | 27.67 |
| ATOM | 1130 | CG  | ASP | A | 160 | 17.981 | 1.620  | 25.873 | 1.00 | 28.84 |
| ATOM | 1131 | OD1 | ASP | A | 160 | 16.776 | 1.290  | 26.014 | 1.00 | 26.79 |
| ATOM | 1132 | OD2 | ASP | A | 160 | 18.735 | 1.597  | 26.865 | 1.00 | 32.92 |
| ATOM | 1133 | C   | ASP | A | 160 | 16.296 | 1.855  | 23.363 | 1.00 | 25.36 |
| ATOM | 1134 | O   | ASP | A | 160 | 15.141 | 2.250  | 23.501 | 1.00 | 23.64 |
| ATOM | 1135 | N   | GLN | A | 161 | 16.614 | 0.641  | 22.915 | 1.00 | 23.95 |
| ATOM | 1136 | CA  | GLN | A | 161 | 15.585 | -0.240 | 22.365 | 1.00 | 24.83 |
| ATOM | 1137 | CB  | GLN | A | 161 | 16.094 | -1.043 | 21.164 | 1.00 | 26.83 |
| ATOM | 1138 | CG  | GLN | A | 161 | 16.563 | -0.146 | 20.012 | 1.00 | 32.67 |
| ATOM | 1139 | CD  | GLN | A | 161 | 16.766 | -0.870 | 18.682 | 1.00 | 42.17 |
| ATOM | 1140 | OE1 | GLN | A | 161 | 16.550 | -2.078 | 18.566 | 1.00 | 44.45 |
| ATOM | 1141 | NE2 | GLN | A | 161 | 17.202 | -0.125 | 17.675 | 1.00 | 44.50 |
| ATOM | 1142 | C   | GLN | A | 161 | 14.907 | -1.126 | 23.415 | 1.00 | 23.64 |
| ATOM | 1143 | O   | GLN | A | 161 | 14.058 | -1.955 | 23.069 | 1.00 | 26.15 |

**FIGURE 274**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1144 | N   | ASP | A | 162 | 15.219 | -0.906 | 24.689 | 1.00 | 21.69 |
| ATOM | 1145 | CA  | ASP | A | 162 | 14.621 | -1.750 | 25.724 | 1.00 | 22.06 |
| ATOM | 1146 | CB  | ASP | A | 162 | 15.416 | -1.717 | 27.025 | 1.00 | 20.34 |
| ATOM | 1147 | CG  | ASP | A | 162 | 16.797 | -2.326 | 26.891 | 1.00 | 29.79 |
| ATOM | 1148 | OD1 | ASP | A | 162 | 17.083 | -2.995 | 25.878 | 1.00 | 31.31 |
| ATOM | 1149 | OD2 | ASP | A | 162 | 17.657 | -2.177 | 27.779 | 1.00 | 39.34 |
| ATOM | 1150 | C   | ASP | A | 162 | 13.240 | -1.174 | 26.011 | 1.00 | 20.10 |
| ATOM | 1151 | O   | ASP | A | 162 | 13.149 | 0.028  | 26.267 | 1.00 | 21.67 |
| ATOM | 1152 | N   | SER | A | 163 | 12.210 | -2.020 | 26.029 | 1.00 | 22.00 |
| ATOM | 1153 | CA  | SER | A | 163 | 10.860 | -1.555 | 26.374 | 1.00 | 19.52 |
| ATOM | 1154 | CB  | SER | A | 163 | 9.797  | -2.621 | 26.127 | 1.00 | 19.81 |
| ATOM | 1155 | OG  | SER | A | 163 | 10.079 | -3.816 | 26.840 | 1.00 | 24.08 |
| ATOM | 1156 | C   | SER | A | 163 | 10.742 | -0.998 | 27.791 | 1.00 | 20.81 |
| ATOM | 1157 | O   | SER | A | 163 | 11.529 | -1.343 | 28.699 | 1.00 | 19.79 |
| ATOM | 1158 | N   | LEU | A | 164 | 9.765  | -0.123 | 27.987 | 1.00 | 20.37 |
| ATOM | 1159 | CA  | LEU | A | 164 | 9.525  | 0.494  | 29.298 | 1.00 | 20.27 |
| ATOM | 1160 | CB  | LEU | A | 164 | 10.225 | 1.847  | 29.418 | 1.00 | 21.91 |
| ATOM | 1161 | CG  | LEU | A | 164 | 11.716 | 2.029  | 29.730 | 1.00 | 28.59 |
| ATOM | 1162 | CD1 | LEU | A | 164 | 11.962 | 3.530  | 29.619 | 1.00 | 32.46 |
| ATOM | 1163 | CD2 | LEU | A | 164 | 11.994 | 1.587  | 31.160 | 1.00 | 29.88 |
| ATOM | 1164 | C   | LEU | A | 164 | 8.031  | 0.814  | 29.392 | 1.00 | 17.64 |
| ATOM | 1165 | O   | LEU | A | 164 | 7.400  | 1.129  | 28.385 | 1.00 | 19.87 |
| ATOM | 1166 | N   | TYR | A | 165 | 7.511  | 0.782  | 30.613 | 1.00 | 18.28 |
| ATOM | 1167 | CA  | TYR | A | 165 | 6.148  | 1.247  | 30.880 | 1.00 | 16.77 |
| ATOM | 1168 | CB  | TYR | A | 165 | 5.625  | 0.605  | 32.160 | 1.00 | 17.12 |
| ATOM | 1169 | CG  | TYR | A | 165 | 4.965  | -0.711 | 31.893 | 1.00 | 20.15 |
| ATOM | 1170 | CD1 | TYR | A | 165 | 3.698  | -0.753 | 31.322 | 1.00 | 21.67 |
| ATOM | 1171 | CE1 | TYR | A | 165 | 3.081  | -1.967 | 31.054 | 1.00 | 19.75 |
| ATOM | 1172 | CZ  | TYR | A | 165 | 3.726  | -3.137 | 31.372 | 1.00 | 23.95 |
| ATOM | 1173 | OH  | TYR | A | 165 | 3.113  | -4.342 | 31.095 | 1.00 | 28.45 |
| ATOM | 1174 | CE2 | TYR | A | 165 | 4.972  | -3.123 | 31.935 | 1.00 | 21.42 |
| ATOM | 1175 | CD2 | TYR | A | 165 | 5.587  | -1.906 | 32.230 | 1.00 | 21.96 |
| ATOM | 1176 | C   | TYR | A | 165 | 6.107  | 2.749  | 31.085 | 1.00 | 19.28 |
| ATOM | 1177 | O   | TYR | A | 165 | 6.948  | 3.318  | 31.778 | 1.00 | 22.32 |
| ATOM | 1178 | N   | TYR | A | 166 | 5.105  | 3.372  | 30.480 | 1.00 | 19.16 |
| ATOM | 1179 | CA  | TYR | A | 166 | 4.668  | 4.714  | 30.858 | 1.00 | 18.90 |
| ATOM | 1180 | CB  | TYR | A | 166 | 4.762  | 5.650  | 29.639 | 1.00 | 19.56 |
| ATOM | 1181 | CG  | TYR | A | 166 | 6.180  | 5.875  | 29.174 | 1.00 | 18.34 |
| ATOM | 1182 | CD1 | TYR | A | 166 | 6.896  | 6.985  | 29.601 | 1.00 | 16.76 |
| ATOM | 1183 | CE1 | TYR | A | 166 | 8.223  | 7.190  | 29.153 | 1.00 | 18.94 |
| ATOM | 1184 | CZ  | TYR | A | 166 | 8.777  | 6.306  | 28.245 | 1.00 | 22.27 |
| ATOM | 1185 | OH  | TYR | A | 166 | 10.067 | 6.497  | 27.780 | 1.00 | 24.37 |
| ATOM | 1186 | CE2 | TYR | A | 166 | 8.067  | 5.222  | 27.789 | 1.00 | 26.25 |
| ATOM | 1187 | CD2 | TYR | A | 166 | 6.768  | 5.016  | 28.245 | 1.00 | 22.49 |
| ATOM | 1188 | C   | TYR | A | 166 | 3.235  | 4.628  | 31.372 | 1.00 | 19.75 |
| ATOM | 1189 | O   | TYR | A | 166 | 2.297  | 4.549  | 30.586 | 1.00 | 20.21 |
| ATOM | 1190 | N   | GLY | A | 167 | 3.032  | 4.609  | 32.694 | 1.00 | 20.43 |
| ATOM | 1191 | CA  | GLY | A | 167 | 1.684  | 4.310  | 33.165 | 1.00 | 21.54 |
| ATOM | 1192 | C   | GLY | A | 167 | 1.209  | 2.931  | 32.728 | 1.00 | 23.50 |
| ATOM | 1193 | O   | GLY | A | 167 | 1.932  | 1.957  | 32.943 | 1.00 | 23.77 |
| ATOM | 1194 | N   | ASP | A | 168 | 0.029  | 2.885  | 32.099 | 1.00 | 21.81 |
| ATOM | 1195 | CA  | ASP | A | 168 | -0.673 | 1.718  | 31.567 | 1.00 | 26.70 |

**FIGURE 275**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1196 | CB  | ASP | A | 168 | -2.086 | 2.171  | 31.152 | 1.00 | 28.49 |
| ATOM | 1197 | CG  | ASP | A | 168 | -3.021 | 2.345  | 32.289 | 1.00 | 35.95 |
| ATOM | 1198 | OD1 | ASP | A | 168 | -2.581 | 2.521  | 33.451 | 1.00 | 44.09 |
| ATOM | 1199 | OD2 | ASP | A | 168 | -4.248 | 2.352  | 32.078 | 1.00 | 36.92 |
| ATOM | 1200 | C   | ASP | A | 168 | -0.150 | 1.270  | 30.206 | 1.00 | 24.58 |
| ATOM | 1201 | O   | ASP | A | 168 | -0.717 | 0.345  | 29.619 | 1.00 | 26.11 |
| ATOM | 1202 | N   | LEU | A | 169 | 0.840  | 1.971  | 29.657 | 1.00 | 21.74 |
| ATOM | 1203 | CA  | LEU | A | 169 | 1.205  | 1.797  | 28.261 | 1.00 | 19.33 |
| ATOM | 1204 | CB  | LEU | A | 169 | 1.174  | 3.152  | 27.567 | 1.00 | 19.99 |
| ATOM | 1205 | CG  | LEU | A | 169 | 1.541  | 3.109  | 26.095 | 1.00 | 25.20 |
| ATOM | 1206 | CD1 | LEU | A | 169 | 0.471  | 3.894  | 25.397 | 1.00 | 26.72 |
| ATOM | 1207 | CD2 | LEU | A | 169 | 2.886  | 3.769  | 25.917 | 1.00 | 25.81 |
| ATOM | 1208 | C   | LEU | A | 169 | 2.619  | 1.256  | 28.197 | 1.00 | 20.65 |
| ATOM | 1209 | O   | LEU | A | 169 | 3.485  | 1.740  | 28.907 | 1.00 | 21.93 |
| ATOM | 1210 | N   | ILE | A | 170 | 2.857  | 0.250  | 27.370 | 1.00 | 18.58 |
| ATOM | 1211 | CA  | ILE | A | 170 | 4.239  | -0.182 | 27.197 | 1.00 | 19.82 |
| ATOM | 1212 | CB  | ILE | A | 170 | 4.309  | -1.728 | 27.237 | 1.00 | 19.31 |
| ATOM | 1213 | CG1 | ILE | A | 170 | 5.746  | -2.220 | 26.983 | 1.00 | 22.75 |
| ATOM | 1214 | CD1 | ILE | A | 170 | 6.454  | -2.519 | 28.252 | 1.00 | 22.15 |
| ATOM | 1215 | CG2 | ILE | A | 170 | 3.367  | -2.344 | 26.238 | 1.00 | 22.33 |
| ATOM | 1216 | C   | ILE | A | 170 | 4.745  | 0.359  | 25.870 | 1.00 | 19.44 |
| ATOM | 1217 | O   | ILE | A | 170 | 4.000  | 0.382  | 24.898 | 1.00 | 19.22 |
| ATOM | 1218 | N   | LEU | A | 171 | 6.009  | 0.775  | 25.817 | 1.00 | 18.90 |
| ATOM | 1219 | CA  | LEU | A | 171 | 6.505  | 1.440  | 24.631 | 1.00 | 18.91 |
| ATOM | 1220 | CB  | LEU | A | 171 | 6.697  | 2.923  | 24.954 | 1.00 | 19.73 |
| ATOM | 1221 | CG  | LEU | A | 171 | 7.108  | 3.758  | 23.751 | 1.00 | 25.25 |
| ATOM | 1222 | CD1 | LEU | A | 171 | 6.670  | 5.162  | 24.054 | 1.00 | 28.25 |
| ATOM | 1223 | CD2 | LEU | A | 171 | 8.618  | 3.703  | 23.723 | 1.00 | 29.29 |
| ATOM | 1224 | C   | LEU | A | 171 | 7.852  | 0.820  | 24.354 | 1.00 | 19.14 |
| ATOM | 1225 | O   | LEU | A | 171 | 8.556  | 0.467  | 25.305 | 1.00 | 18.74 |
| ATOM | 1226 | N   | GLN | A | 172 | 8.174  | 0.655  | 23.074 | 1.00 | 17.00 |
| ATOM | 1227 | CA  | GLN | A | 172 | 9.485  | 0.117  | 22.713 | 1.00 | 18.63 |
| ATOM | 1228 | CB  | GLN | A | 172 | 9.392  | -1.379 | 22.439 | 1.00 | 19.29 |
| ATOM | 1229 | CG  | GLN | A | 172 | 10.724 | -2.109 | 22.277 | 1.00 | 25.23 |
| ATOM | 1230 | CD  | GLN | A | 172 | 10.473 | -3.552 | 21.842 | 1.00 | 28.98 |
| ATOM | 1231 | OE1 | GLN | A | 172 | 9.779  | -3.776 | 20.859 | 1.00 | 30.54 |
| ATOM | 1232 | NE2 | GLN | A | 172 | 11.024 | -4.521 | 22.559 | 1.00 | 24.05 |
| ATOM | 1233 | C   | GLN | A | 172 | 9.946  | 0.820  | 21.464 | 1.00 | 17.56 |
| ATOM | 1234 | O   | GLN | A | 172 | 9.242  | 0.825  | 20.460 | 1.00 | 20.89 |
| ATOM | 1235 | N   | MET | A | 173 | 11.166 | 1.337  | 21.506 | 1.00 | 18.09 |
| ATOM | 1236 | CA  | MET | A | 173 | 11.703 | 2.006  | 20.315 | 1.00 | 19.64 |
| ATOM | 1237 | CB  | MET | A | 173 | 12.860 | 2.934  | 20.713 | 1.00 | 15.61 |
| ATOM | 1238 | CG  | MET | A | 173 | 13.415 | 3.696  | 19.493 | 1.00 | 20.90 |
| ATOM | 1239 | SD  | MET | A | 173 | 14.248 | 5.251  | 19.921 | 1.00 | 22.90 |
| ATOM | 1240 | CE  | MET | A | 173 | 15.666 | 4.695  | 20.787 | 1.00 | 24.34 |
| ATOM | 1241 | C   | MET | A | 173 | 12.262 | 0.942  | 19.386 | 1.00 | 20.45 |
| ATOM | 1242 | O   | MET | A | 173 | 13.189 | 0.219  | 19.790 | 1.00 | 23.02 |
| ATOM | 1243 | N   | LEU | A | 174 | 11.783 | 0.916  | 18.144 | 1.00 | 19.05 |
| ATOM | 1244 | CA  | LEU | A | 174 | 12.245 | -0.028 | 17.131 | 1.00 | 20.65 |
| ATOM | 1245 | CB  | LEU | A | 174 | 11.102 | -0.481 | 16.243 | 1.00 | 22.05 |
| ATOM | 1246 | CG  | LEU | A | 174 | 9.874  | -1.071 | 16.934 | 1.00 | 19.97 |
| ATOM | 1247 | CD1 | LEU | A | 174 | 8.825  | -1.459 | 15.899 | 1.00 | 25.97 |

**FIGURE 276**



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1248 | CD2 | LEU | A | 174 | 10.205 | -2.246 | 17.825 | 1.00 | 24.09 |
| ATOM | 1249 | C   | LEU | A | 174 | 13.385 | 0.487  | 16.262 | 1.00 | 22.40 |
| ATOM | 1250 | O   | LEU | A | 174 | 14.226 | -0.290 | 15.807 | 1.00 | 23.87 |
| ATOM | 1251 | N   | SER | A | 175 | 13.419 | 1.794  | 16.031 | 1.00 | 21.05 |
| ATOM | 1252 | CA  | SER | A | 175 | 14.501 | 2.374  | 15.250 | 1.00 | 20.96 |
| ATOM | 1253 | CB  | SER | A | 175 | 14.261 | 2.317  | 13.743 | 1.00 | 19.89 |
| ATOM | 1254 | OG  | SER | A | 175 | 13.038 | 2.900  | 13.345 | 1.00 | 21.43 |
| ATOM | 1255 | C   | SER | A | 175 | 14.670 | 3.819  | 15.645 | 1.00 | 18.88 |
| ATOM | 1256 | O   | SER | A | 175 | 13.739 | 4.466  | 16.097 | 1.00 | 19.35 |
| ATOM | 1257 | N   | GLU | A | 176 | 15.880 | 4.300  | 15.439 | 1.00 | 17.31 |
| ATOM | 1258 | CA  | GLU | A | 176 | 16.187 | 5.707  | 15.592 | 1.00 | 17.56 |
| ATOM | 1259 | CB  | GLU | A | 176 | 16.755 | 5.907  | 16.988 | 1.00 | 19.24 |
| ATOM | 1260 | CG  | GLU | A | 176 | 17.299 | 7.278  | 17.319 | 1.00 | 22.48 |
| ATOM | 1261 | CD  | GLU | A | 176 | 17.792 | 7.337  | 18.749 | 1.00 | 24.54 |
| ATOM | 1262 | OE1 | GLU | A | 176 | 18.951 | 6.933  | 19.003 | 1.00 | 35.75 |
| ATOM | 1263 | OE2 | GLU | A | 176 | 17.050 | 7.813  | 19.612 | 1.00 | 25.21 |
| ATOM | 1264 | C   | GLU | A | 176 | 17.141 | 6.067  | 14.463 | 1.00 | 17.07 |
| ATOM | 1265 | O   | GLU | A | 176 | 18.276 | 5.559  | 14.397 | 1.00 | 19.83 |
| ATOM | 1266 | N   | SER | A | 177 | 16.684 | 6.953  | 13.579 | 1.00 | 18.92 |
| ATOM | 1267 | CA  | SER | A | 177 | 17.484 | 7.339  | 12.419 | 1.00 | 20.17 |
| ATOM | 1268 | CB  | SER | A | 177 | 16.766 | 6.925  | 11.139 | 1.00 | 19.64 |
| ATOM | 1269 | OG  | SER | A | 177 | 16.378 | 5.553  | 11.196 | 1.00 | 26.41 |
| ATOM | 1270 | C   | SER | A | 177 | 17.786 | 8.844  | 12.477 | 1.00 | 18.07 |
| ATOM | 1271 | O   | SER | A | 177 | 16.922 | 9.671  | 12.295 | 1.00 | 16.18 |
| ATOM | 1272 | N   | VAL | A | 178 | 19.035 | 9.210  | 12.728 | 1.00 | 19.19 |
| ATOM | 1273 | CA  | VAL | A | 178 | 19.408 | 10.605 | 12.863 | 1.00 | 18.44 |
| ATOM | 1274 | CB  | VAL | A | 178 | 20.648 | 10.758 | 13.802 | 1.00 | 18.96 |
| ATOM | 1275 | CG1 | VAL | A | 178 | 21.063 | 12.211 | 13.900 | 1.00 | 19.33 |
| ATOM | 1276 | CG2 | VAL | A | 178 | 20.350 | 10.128 | 15.180 | 1.00 | 22.08 |
| ATOM | 1277 | C   | VAL | A | 178 | 19.814 | 11.098 | 11.472 | 1.00 | 17.78 |
| ATOM | 1278 | O   | VAL | A | 178 | 20.753 | 10.578 | 10.850 | 1.00 | 18.38 |
| ATOM | 1279 | N   | LEU | A | 179 | 19.070 | 12.075 | 10.970 | 1.00 | 18.02 |
| ATOM | 1280 | CA  | LEU | A | 179 | 19.347 | 12.663 | 9.663  | 1.00 | 16.64 |
| ATOM | 1281 | CB  | LEU | A | 179 | 18.074 | 12.673 | 8.777  | 1.00 | 17.91 |
| ATOM | 1282 | CG  | LEU | A | 179 | 17.193 | 11.405 | 8.899  | 1.00 | 18.10 |
| ATOM | 1283 | CD1 | LEU | A | 179 | 15.925 | 11.510 | 8.066  | 1.00 | 18.94 |
| ATOM | 1284 | CD2 | LEU | A | 179 | 17.912 | 10.091 | 8.610  | 1.00 | 15.53 |
| ATOM | 1285 | C   | LEU | A | 179 | 19.922 | 14.059 | 9.914  | 1.00 | 17.92 |
| ATOM | 1286 | O   | LEU | A | 179 | 20.078 | 14.486 | 11.066 | 1.00 | 18.05 |
| ATOM | 1287 | N   | PRO | A | 180 | 20.307 | 14.764 | 8.862  | 1.00 | 15.89 |
| ATOM | 1288 | CA  | PRO | A | 180 | 20.946 | 16.077 | 9.031  | 1.00 | 17.67 |
| ATOM | 1289 | CB  | PRO | A | 180 | 21.055 | 16.593 | 7.609  | 1.00 | 16.61 |
| ATOM | 1290 | CG  | PRO | A | 180 | 21.283 | 15.311 | 6.840  | 1.00 | 17.50 |
| ATOM | 1291 | CD  | PRO | A | 180 | 20.255 | 14.354 | 7.454  | 1.00 | 16.79 |
| ATOM | 1292 | C   | PRO | A | 180 | 20.190 | 17.085 | 9.863  | 1.00 | 17.87 |
| ATOM | 1293 | O   | PRO | A | 180 | 20.802 | 17.756 | 10.702 | 1.00 | 19.82 |
| ATOM | 1294 | N   | GLU | A | 181 | 18.878 | 17.189 | 9.656  | 1.00 | 17.72 |
| ATOM | 1295 | CA  | GLU | A | 181 | 18.130 | 18.231 | 10.335 | 1.00 | 19.40 |
| ATOM | 1296 | CB  | GLU | A | 181 | 17.737 | 19.349 | 9.366  | 1.00 | 20.16 |
| ATOM | 1297 | CG  | GLU | A | 181 | 18.973 | 20.058 | 8.833  | 1.00 | 24.30 |
| ATOM | 1298 | CD  | GLU | A | 181 | 18.615 | 21.064 | 7.765  | 1.00 | 30.86 |
| ATOM | 1299 | OE1 | GLU | A | 181 | 17.597 | 20.866 | 7.057  | 1.00 | 33.00 |

**FIGURE 277**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1300 | OE2 | GLU | A | 181 | 19.384 | 22.040 | 7.641  | 1.00 | 39.73 |
| ATOM | 1301 | C   | GLU | A | 181 | 16.890 | 17.704 | 11.048 | 1.00 | 19.38 |
| ATOM | 1302 | O   | GLU | A | 181 | 16.209 | 18.470 | 11.692 | 1.00 | 19.21 |
| ATOM | 1303 | N   | TRP | A | 182 | 16.619 | 16.405 | 10.942 | 1.00 | 16.49 |
| ATOM | 1304 | CA  | TRP | A | 182 | 15.667 | 15.784 | 11.836 | 1.00 | 16.57 |
| ATOM | 1305 | CB  | TRP | A | 182 | 14.242 | 15.924 | 11.286 | 1.00 | 15.22 |
| ATOM | 1306 | CG  | TRP | A | 182 | 14.026 | 15.548 | 9.833  | 1.00 | 13.61 |
| ATOM | 1307 | CD1 | TRP | A | 182 | 13.615 | 14.342 | 9.354  | 1.00 | 15.76 |
| ATOM | 1308 | NE1 | TRP | A | 182 | 13.472 | 14.385 | 7.987  | 1.00 | 16.34 |
| ATOM | 1309 | CE2 | TRP | A | 182 | 13.726 | 15.663 | 7.565  | 1.00 | 13.66 |
| ATOM | 1310 | CD2 | TRP | A | 182 | 14.072 | 16.427 | 8.713  | 1.00 | 14.52 |
| ATOM | 1311 | CE3 | TRP | A | 182 | 14.416 | 17.767 | 8.547  | 1.00 | 16.17 |
| ATOM | 1312 | CZ3 | TRP | A | 182 | 14.369 | 18.307 | 7.265  | 1.00 | 17.28 |
| ATOM | 1313 | CH2 | TRP | A | 182 | 14.019 | 17.520 | 6.154  | 1.00 | 20.20 |
| ATOM | 1314 | CZ2 | TRP | A | 182 | 13.697 | 16.196 | 6.281  | 1.00 | 18.18 |
| ATOM | 1315 | C   | TRP | A | 182 | 16.019 | 14.330 | 12.118 | 1.00 | 17.43 |
| ATOM | 1316 | O   | TRP | A | 182 | 16.831 | 13.721 | 11.423 | 1.00 | 16.83 |
| ATOM | 1317 | N   | THR | A | 183 | 15.372 | 13.776 | 13.135 | 1.00 | 17.91 |
| ATOM | 1318 | CA  | THR | A | 183 | 15.570 | 12.391 | 13.524 | 1.00 | 17.41 |
| ATOM | 1319 | CB  | THR | A | 183 | 16.158 | 12.387 | 14.941 | 1.00 | 17.91 |
| ATOM | 1320 | OG1 | THR | A | 183 | 17.508 | 12.889 | 14.867 | 1.00 | 19.93 |
| ATOM | 1321 | CG2 | THR | A | 183 | 16.379 | 10.952 | 15.444 | 1.00 | 19.10 |
| ATOM | 1322 | C   | THR | A | 183 | 14.216 | 11.704 | 13.494 | 1.00 | 18.88 |
| ATOM | 1323 | O   | THR | A | 183 | 13.253 | 12.259 | 14.020 | 1.00 | 17.96 |
| ATOM | 1324 | N   | ILE | A | 184 | 14.159 | 10.521 | 12.884 | 1.00 | 14.76 |
| ATOM | 1325 | CA  | ILE | A | 184 | 12.915 | 9.770  | 12.795 | 1.00 | 15.33 |
| ATOM | 1326 | CB  | ILE | A | 184 | 12.636 | 9.313  | 11.362 | 1.00 | 15.60 |
| ATOM | 1327 | CG1 | ILE | A | 184 | 12.620 | 10.508 | 10.410 | 1.00 | 14.39 |
| ATOM | 1328 | CD1 | ILE | A | 184 | 12.371 | 10.133 | 8.960  | 1.00 | 16.80 |
| ATOM | 1329 | CG2 | ILE | A | 184 | 11.318 | 8.518  | 11.307 | 1.00 | 18.05 |
| ATOM | 1330 | C   | ILE | A | 184 | 13.050 | 8.539  | 13.682 | 1.00 | 16.19 |
| ATOM | 1331 | O   | ILE | A | 184 | 13.965 | 7.725  | 13.524 | 1.00 | 18.12 |
| ATOM | 1332 | N   | ARG | A | 185 | 12.106 | 8.368  | 14.592 | 1.00 | 16.20 |
| ATOM | 1333 | CA  | ARG | A | 185 | 12.083 | 7.159  | 15.425 | 1.00 | 15.84 |
| ATOM | 1334 | CB  | ARG | A | 185 | 12.137 | 7.551  | 16.904 | 1.00 | 14.71 |
| ATOM | 1335 | CG  | ARG | A | 185 | 13.505 | 8.055  | 17.326 | 1.00 | 14.82 |
| ATOM | 1336 | CD  | ARG | A | 185 | 13.468 | 8.727  | 18.685 | 1.00 | 17.62 |
| ATOM | 1337 | NE  | ARG | A | 185 | 14.822 | 9.174  | 19.013 | 1.00 | 21.26 |
| ATOM | 1338 | CZ  | ARG | A | 185 | 15.195 | 10.448 | 18.973 | 1.00 | 21.83 |
| ATOM | 1339 | NH1 | ARG | A | 185 | 14.345 | 11.379 | 18.584 | 1.00 | 21.65 |
| ATOM | 1340 | NH2 | ARG | A | 185 | 16.422 | 10.807 | 19.323 | 1.00 | 26.56 |
| ATOM | 1341 | C   | ARG | A | 185 | 10.808 | 6.386  | 15.181 | 1.00 | 16.96 |
| ATOM | 1342 | O   | ARG | A | 185 | 9.775  | 6.967  | 14.866 | 1.00 | 18.49 |
| ATOM | 1343 | N   | GLU | A | 186 | 10.876 | 5.063  | 15.330 | 1.00 | 18.06 |
| ATOM | 1344 | CA  | GLU | A | 186 | 9.653  | 4.289  | 15.251 | 1.00 | 18.19 |
| ATOM | 1345 | CB  | GLU | A | 186 | 9.729  | 3.232  | 14.126 | 1.00 | 18.51 |
| ATOM | 1346 | CG  | GLU | A | 186 | 8.354  | 2.622  | 13.856 | 1.00 | 22.77 |
| ATOM | 1347 | CD  | GLU | A | 186 | 8.367  | 1.477  | 12.851 | 1.00 | 31.07 |
| ATOM | 1348 | OE1 | GLU | A | 186 | 7.330  | 1.279  | 12.179 | 1.00 | 37.68 |
| ATOM | 1349 | OE2 | GLU | A | 186 | 9.388  | 0.775  | 12.730 | 1.00 | 33.77 |
| ATOM | 1350 | C   | GLU | A | 186 | 9.452  | 3.600  | 16.597 | 1.00 | 18.63 |
| ATOM | 1351 | O   | GLU | A | 186 | 10.411 | 3.051  | 17.142 | 1.00 | 19.33 |

FIGURE 278

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Three Dimensional Coordinates of HPTPbeta

|      |      |         |     |     |       |        |        |        |       |       |
|------|------|---------|-----|-----|-------|--------|--------|--------|-------|-------|
| ATOM | 1352 | N       | PHE | A   | 187   | 8.223  | 3.614  | 17.108 | 1.00  | 18.68 |
| ATOM | 1353 | CA      | PHE | A   | 187   | 7.927  | 2.978  | 18.399 | 1.00  | 18.08 |
| ATOM | 1354 | CB      | PHE | A   | 187   | 7.426  | 4.006  | 19.415 | 1.00  | 18.99 |
| ATOM | 1355 | CG      | PHE | A   | 187   | 8.400  | 5.092  | 19.715 | 1.00  | 19.80 |
| ATOM | 1356 | CD1     | PHE | A   | 187   | 8.155  | 6.382  | 19.283 | 1.00  | 21.67 |
| ATOM | 1357 | CE1     | PHE | A   | 187   | 9.066  | 7.403  | 19.559 | 1.00  | 23.38 |
| ATOM | 1358 | CZ      | PHE | A   | 187   | 10.242 | 7.106  | 20.223 | 1.00  | 20.03 |
| ATOM | 1359 | CE2     | PHE | A   | 187   | 10.489 | 5.828  | 20.641 | 1.00  | 25.29 |
| ATOM | 1360 | CD2     | PHE | A   | 187   | 9.595  | 4.819  | 20.369 | 1.00  | 22.12 |
| ATOM | 1361 | C       | PHE | A   | 187   | 6.815  | 1.954  | 18.257 | 1.00  | 19.06 |
| ATOM | 1362 | O       | PHE | A   | 187   | 5.881  | 2.161  | 17.472 | 1.00  | 18.23 |
| ATOM | 1363 | N       | LYS | A   | 188   | 6.898  | 0.863  | 19.018 | 1.00  | 18.39 |
| ATOM | 1364 | CA      | LYS | A   | 188   | 5.718  | 0.006  | 19.179 | 1.00  | 19.84 |
| ATOM | 1365 | CB      | LYS | A   | 188   | 6.146  | -1.466 | 19.179 | 1.00  | 21.30 |
| ATOM | 1366 | CG      | LYS | A   | 188   | 4.994  | -2.449 | 19.361 | 1.00  | 29.28 |
| ATOM | 1367 | CD      | LYS | A   | 188   | 5.549  | -3.835 | 19.650 | 1.00  | 39.42 |
| ATOM | 1368 | CE      | LYS | A   | 188   | 4.535  | -4.915 | 19.312 | 1.00  | 41.60 |
| ATOM | 1369 | NZ      | LYS | A   | 188   | 5.247  | -6.141 | 18.830 | 1.00  | 47.94 |
| ATOM | 1370 | C       | LYS | A   | 188   | 5.076  | 0.377  | 20.513 | 1.00  | 17.53 |
| ATOM | 1371 | O       | LYS | A   | 188   | 5.765  | 0.472  | 21.511 | 1.00  | 20.08 |
| ATOM | 1372 | N       | ILE | A   | 189   | 3.761  | 0.584  | 20.551 | 1.00  | 18.34 |
| ATOM | 1373 | CA      | ILE | A   | 189   | 3.063  | 0.924  | 21.781 | 1.00  | 18.37 |
| ATOM | 1374 | CB      | ILE | A   | 189   | 2.662  | 2.409  | 21.729 | 1.00  | 17.71 |
| ATOM | 1375 | CG1AILE | A   | 189 | 2.140 | 2.932  | 23.051 | 0.50   | 18.61 |       |
| ATOM | 1376 | CG1BILE | A   | 189 | 1.794 | 2.771  | 20.521 | 0.50   | 19.99 |       |
| ATOM | 1377 | CD1AILE | A   | 189 | 1.758 | 4.385  | 22.938 | 0.50   | 20.42 |       |
| ATOM | 1378 | CD1BILE | A   | 189 | 1.063 | 4.085  | 20.730 | 0.50   | 24.91 |       |
| ATOM | 1379 | CG2AILE | A   | 189 | 1.579 | 2.616  | 20.661 | 0.50   | 18.62 |       |
| ATOM | 1380 | CG2BILE | A   | 189 | 3.921 | 3.269  | 21.880 | 0.50   | 16.15 |       |
| ATOM | 1381 | C       | ILE | A   | 189   | 1.848  | -0.013 | 21.922 | 1.00  | 17.83 |
| ATOM | 1382 | O       | ILE | A   | 189   | 1.239  | -0.400 | 20.918 | 1.00  | 16.89 |
| ATOM | 1383 | N       | CYS | A   | 190   | 1.567  | -0.403 | 23.165 | 1.00  | 19.24 |
| ATOM | 1384 | CA      | CYS | A   | 190   | 0.313  | -1.068 | 23.547 | 1.00  | 19.00 |
| ATOM | 1385 | CB      | CYS | A   | 190   | 0.590  | -2.542 | 23.881 | 1.00  | 17.53 |
| ATOM | 1386 | SG      | CYS | A   | 190   | 1.496  | -3.470 | 22.591 | 1.00  | 25.53 |
| ATOM | 1387 | C       | CYS | A   | 190   | -0.258 | -0.402 | 24.791 | 1.00  | 18.76 |
| ATOM | 1388 | O       | CYS | A   | 190   | 0.428  | -0.293 | 25.789 | 1.00  | 18.93 |
| ATOM | 1389 | N       | GLY | A   | 191   | -1.534 | -0.004 | 24.757 | 1.00  | 18.32 |
| ATOM | 1390 | CA      | GLY | A   | 191   | -2.213 | 0.527  | 25.930 | 1.00  | 20.25 |
| ATOM | 1391 | C       | GLY | A   | 191   | -3.530 | -0.202 | 26.162 | 1.00  | 20.72 |
| ATOM | 1392 | O       | GLY | A   | 191   | -3.740 | -1.262 | 25.606 | 1.00  | 20.46 |
| ATOM | 1393 | N       | GLU | A   | 192   | -4.386 | 0.359  | 27.002 | 1.00  | 22.42 |
| ATOM | 1394 | CA      | GLU | A   | 192   | -5.677 | -0.253 | 27.279 | 1.00  | 24.91 |
| ATOM | 1395 | CB      | GLU | A   | 192   | -6.421 | 0.585  | 28.315 | 1.00  | 23.09 |
| ATOM | 1396 | CG      | GLU | A   | 192   | -7.854 | 0.111  | 28.537 | 1.00  | 29.54 |
| ATOM | 1397 | CD      | GLU | A   | 192   | -8.646 | 0.961  | 29.512 | 1.00  | 32.49 |
| ATOM | 1398 | OE1     | GLU | A   | 192   | -8.290 | 2.150  | 29.745 | 1.00  | 31.32 |
| ATOM | 1399 | OE2     | GLU | A   | 192   | -9.661 | 0.426  | 30.018 | 1.00  | 34.67 |
| ATOM | 1400 | C       | GLU | A   | 192   | -6.461 | -0.414 | 25.974 | 1.00  | 24.14 |
| ATOM | 1401 | O       | GLU | A   | 192   | -6.810 | 0.567  | 25.289 | 1.00  | 24.16 |
| ATOM | 1402 | N       | GLU | A   | 193   | -6.719 | -1.671 | 25.612 | 1.00  | 25.67 |
| ATOM | 1403 | CA      | GLU | A   | 193   | -7.236 | -1.978 | 24.284 | 1.00  | 26.65 |

**FIGURE 279**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |         |        |        |      |       |
|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 1404 | CB  | GLU | A | 193 | -7.337  | -3.489 | 24.068 | 1.00 | 28.45 |
| ATOM | 1405 | CG  | GLU | A | 193 | -7.767  | -3.843 | 22.648 | 1.00 | 29.15 |
| ATOM | 1406 | CD  | GLU | A | 193 | -7.780  | -5.342 | 22.405 | 1.00 | 34.41 |
| ATOM | 1407 | OE1 | GLU | A | 193 | -7.163  | -6.077 | 23.211 | 1.00 | 33.00 |
| ATOM | 1408 | OE2 | GLU | A | 193 | -8.400  | -5.778 | 21.408 | 1.00 | 34.70 |
| ATOM | 1409 | C   | GLU | A | 193 | -8.598  | -1.366 | 24.010 | 1.00 | 30.04 |
| ATOM | 1410 | O   | GLU | A | 193 | -9.510  | -1.555 | 24.810 | 1.00 | 29.04 |
| ATOM | 1411 | N   | GLN | A | 194 | -8.730  | -0.635 | 22.902 | 1.00 | 28.72 |
| ATOM | 1412 | CA  | GLN | A | 194 | -10.054 | -0.254 | 22.417 | 1.00 | 30.57 |
| ATOM | 1413 | CB  | GLN | A | 194 | -10.349 | 1.229  | 22.654 | 1.00 | 30.30 |
| ATOM | 1414 | CG  | GLN | A | 194 | -10.354 | 1.700  | 24.097 | 1.00 | 38.21 |
| ATOM | 1415 | CD  | GLN | A | 194 | -10.661 | 3.192  | 24.205 | 1.00 | 45.81 |
| ATOM | 1416 | OE1 | GLN | A | 194 | -11.766 | 3.629  | 23.868 | 1.00 | 47.74 |
| ATOM | 1417 | NE2 | GLN | A | 194 | -9.682  | 3.976  | 24.667 | 1.00 | 48.46 |
| ATOM | 1418 | C   | GLN | A | 194 | -10.138 | -0.612 | 20.937 | 1.00 | 30.81 |
| ATOM | 1419 | O   | GLN | A | 194 | -10.444 | -1.762 | 20.596 | 1.00 | 31.43 |
| ATOM | 1420 | N   | LEU | A | 195 | -9.843  | 0.343  | 20.056 | 1.00 | 30.77 |
| ATOM | 1421 | CA  | LEU | A | 195 | -9.869  | 0.103  | 18.620 | 1.00 | 31.53 |
| ATOM | 1422 | CB  | LEU | A | 195 | -9.860  | 1.419  | 17.833 | 1.00 | 32.19 |
| ATOM | 1423 | CG  | LEU | A | 195 | -11.132 | 2.254  | 17.673 | 1.00 | 37.67 |
| ATOM | 1424 | CD1 | LEU | A | 195 | -10.860 | 3.277  | 16.579 | 1.00 | 33.54 |
| ATOM | 1425 | CD2 | LEU | A | 195 | -12.359 | 1.404  | 17.322 | 1.00 | 36.45 |
| ATOM | 1426 | C   | LEU | A | 195 | -8.692  | -0.729 | 18.144 | 1.00 | 31.71 |
| ATOM | 1427 | O   | LEU | A | 195 | -8.796  | -1.454 | 17.159 | 1.00 | 32.54 |
| ATOM | 1428 | N   | ASP | A | 196 | -7.554  | -0.607 | 18.821 | 1.00 | 29.57 |
| ATOM | 1429 | CA  | ASP | A | 196 | -6.442  | -1.492 | 18.533 | 1.00 | 28.34 |
| ATOM | 1430 | CB  | ASP | A | 196 | -5.424  | -0.868 | 17.558 | 1.00 | 26.58 |
| ATOM | 1431 | CG  | ASP | A | 196 | -4.815  | 0.420  | 18.063 | 1.00 | 27.01 |
| ATOM | 1432 | OD1 | ASP | A | 196 | -5.145  | 0.869  | 19.183 | 1.00 | 27.13 |
| ATOM | 1433 | OD2 | ASP | A | 196 | -3.989  | 1.049  | 17.375 | 1.00 | 25.88 |
| ATOM | 1434 | C   | ASP | A | 196 | -5.791  | -2.008 | 19.815 | 1.00 | 27.72 |
| ATOM | 1435 | O   | ASP | A | 196 | -6.099  | -1.550 | 20.915 | 1.00 | 26.99 |
| ATOM | 1436 | N   | ALA | A | 197 | -4.912  | -2.989 | 19.653 | 1.00 | 26.66 |
| ATOM | 1437 | CA  | ALA | A | 197 | -4.279  | -3.646 | 20.792 | 1.00 | 26.48 |
| ATOM | 1438 | CB  | ALA | A | 197 | -4.557  | -5.145 | 20.748 | 1.00 | 27.66 |
| ATOM | 1439 | C   | ALA | A | 197 | -2.774  | -3.400 | 20.744 | 1.00 | 24.78 |
| ATOM | 1440 | O   | ALA | A | 197 | -2.122  | -3.483 | 21.779 | 1.00 | 26.10 |
| ATOM | 1441 | N   | HIS | A | 198 | -2.237  | -3.062 | 19.573 | 1.00 | 23.60 |
| ATOM | 1442 | CA  | HIS | A | 198 | -0.811  | -2.715 | 19.465 | 1.00 | 24.08 |
| ATOM | 1443 | CB  | HIS | A | 198 | 0.098   | -3.951 | 19.353 | 1.00 | 26.63 |
| ATOM | 1444 | CG  | HIS | A | 198 | -0.227  | -4.848 | 18.198 | 1.00 | 31.90 |
| ATOM | 1445 | ND1 | HIS | A | 198 | -1.094  | -5.914 | 18.300 | 1.00 | 40.11 |
| ATOM | 1446 | CE1 | HIS | A | 198 | -1.186  | -6.519 | 17.128 | 1.00 | 38.77 |
| ATOM | 1447 | NE2 | HIS | A | 198 | -0.406  | -5.886 | 16.271 | 1.00 | 43.28 |
| ATOM | 1448 | CD2 | HIS | A | 198 | 0.215   | -4.844 | 16.918 | 1.00 | 33.37 |
| ATOM | 1449 | C   | HIS | A | 198 | -0.679  | -1.841 | 18.217 | 1.00 | 22.55 |
| ATOM | 1450 | O   | HIS | A | 198 | -1.523  | -1.964 | 17.329 | 1.00 | 24.31 |
| ATOM | 1451 | N   | ARG | A | 199 | 0.343   | -0.980 | 18.167 | 1.00 | 20.23 |
| ATOM | 1452 | CA  | ARG | A | 199 | 0.416   | 0.062  | 17.138 | 1.00 | 18.98 |
| ATOM | 1453 | CB  | ARG | A | 199 | -0.341  | 1.295  | 17.651 | 1.00 | 17.45 |
| ATOM | 1454 | CG  | ARG | A | 199 | -0.566  | 2.347  | 16.560 | 1.00 | 19.76 |
| ATOM | 1455 | CD  | ARG | A | 199 | -1.165  | 3.621  | 17.129 | 1.00 | 19.36 |

**FIGURE 280**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1456 | NE  | ARG | A | 199 | -2.420 | 3.326  | 17.842 | 1.00 | 18.91 |
| ATOM | 1457 | CZ  | ARG | A | 199 | -2.944 | 4.092  | 18.798 | 1.00 | 18.52 |
| ATOM | 1458 | NH1 | ARG | A | 199 | -2.381 | 5.247  | 19.087 | 1.00 | 17.08 |
| ATOM | 1459 | NH2 | ARG | A | 199 | -4.066 | 3.733  | 19.428 | 1.00 | 19.74 |
| ATOM | 1460 | C   | ARG | A | 199 | 1.858  | 0.488  | 16.894 | 1.00 | 19.23 |
| ATOM | 1461 | O   | ARG | A | 199 | 2.642  | 0.507  | 17.836 | 1.00 | 20.70 |
| ATOM | 1462 | N   | LEU | A | 200 | 2.183  | 0.809  | 15.639 | 1.00 | 19.23 |
| ATOM | 1463 | CA  | LEU | A | 200 | 3.472  | 1.424  | 15.309 | 1.00 | 21.60 |
| ATOM | 1464 | CB  | LEU | A | 200 | 4.021  | 0.867  | 13.984 | 1.00 | 22.49 |
| ATOM | 1465 | CG  | LEU | A | 200 | 4.201  | -0.647 | 13.999 | 1.00 | 27.67 |
| ATOM | 1466 | CD1 | LEU | A | 200 | 4.779  | -1.119 | 12.672 | 1.00 | 28.09 |
| ATOM | 1467 | CD2 | LEU | A | 200 | 5.160  | -1.011 | 15.130 | 1.00 | 28.54 |
| ATOM | 1468 | C   | LEU | A | 200 | 3.225  | 2.920  | 15.166 | 1.00 | 21.95 |
| ATOM | 1469 | O   | LEU | A | 200 | 2.245  | 3.324  | 14.521 | 1.00 | 24.40 |
| ATOM | 1470 | N   | ILE | A | 201 | 4.088  | 3.707  | 15.798 | 1.00 | 19.67 |
| ATOM | 1471 | CA  | ILE | A | 201 | 4.022  | 5.165  | 15.845 | 1.00 | 22.82 |
| ATOM | 1472 | CB  | ILE | A | 201 | 4.095  | 5.679  | 17.309 | 1.00 | 24.19 |
| ATOM | 1473 | CG1 | ILE | A | 201 | 2.877  | 5.227  | 18.090 | 1.00 | 31.22 |
| ATOM | 1474 | CD1 | ILE | A | 201 | 1.753  | 4.981  | 17.178 | 1.00 | 26.82 |
| ATOM | 1475 | CG2 | ILE | A | 201 | 4.104  | 7.245  | 17.358 | 1.00 | 27.78 |
| ATOM | 1476 | C   | ILE | A | 201 | 5.295  | 5.667  | 15.190 | 1.00 | 20.99 |
| ATOM | 1477 | O   | ILE | A | 201 | 6.374  | 5.155  | 15.492 | 1.00 | 21.91 |
| ATOM | 1478 | N   | ARG | A | 202 | 5.216  | 6.709  | 14.376 | 1.00 | 19.22 |
| ATOM | 1479 | CA  | ARG | A | 202 | 6.473  | 7.346  | 13.949 | 1.00 | 18.14 |
| ATOM | 1480 | CB  | ARG | A | 202 | 6.517  | 7.524  | 12.440 | 1.00 | 19.80 |
| ATOM | 1481 | CG  | ARG | A | 202 | 6.696  | 6.213  | 11.693 | 1.00 | 25.47 |
| ATOM | 1482 | CD  | ARG | A | 202 | 7.194  | 6.457  | 10.291 | 1.00 | 32.91 |
| ATOM | 1483 | NE  | ARG | A | 202 | 7.555  | 5.237  | 9.577  | 1.00 | 38.14 |
| ATOM | 1484 | CZ  | ARG | A | 202 | 8.719  | 4.609  | 9.709  | 1.00 | 43.78 |
| ATOM | 1485 | NH1 | ARG | A | 202 | 9.646  | 5.051  | 10.552 | 1.00 | 42.73 |
| ATOM | 1486 | NH2 | ARG | A | 202 | 8.964  | 3.520  | 8.994  | 1.00 | 45.94 |
| ATOM | 1487 | C   | ARG | A | 202 | 6.600  | 8.705  | 14.639 | 1.00 | 18.39 |
| ATOM | 1488 | O   | ARG | A | 202 | 5.591  | 9.334  | 14.917 | 1.00 | 19.31 |
| ATOM | 1489 | N   | HIS | A | 203 | 7.829  | 9.072  | 14.982 | 1.00 | 17.24 |
| ATOM | 1490 | CA  | HIS | A | 203 | 8.142  | 10.319 | 15.694 | 1.00 | 16.77 |
| ATOM | 1491 | CB  | HIS | A | 203 | 8.729  | 9.943  | 17.068 | 1.00 | 16.74 |
| ATOM | 1492 | CG  | HIS | A | 203 | 8.980  | 11.095 | 17.996 | 1.00 | 17.60 |
| ATOM | 1493 | ND1 | HIS | A | 203 | 10.173 | 11.794 | 18.011 | 1.00 | 18.12 |
| ATOM | 1494 | CE1 | HIS | A | 203 | 10.133 | 12.706 | 18.970 | 1.00 | 17.49 |
| ATOM | 1495 | NE2 | HIS | A | 203 | 8.946  | 12.647 | 19.552 | 1.00 | 17.63 |
| ATOM | 1496 | CD2 | HIS | A | 203 | 8.221  | 11.629 | 18.985 | 1.00 | 18.26 |
| ATOM | 1497 | C   | HIS | A | 203 | 9.178  | 11.090 | 14.880 | 1.00 | 16.45 |
| ATOM | 1498 | O   | HIS | A | 203 | 10.257 | 10.574 | 14.537 | 1.00 | 16.92 |
| ATOM | 1499 | N   | PHE | A | 204 | 8.811  | 12.326 | 14.542 | 1.00 | 17.22 |
| ATOM | 1500 | CA  | PHE | A | 204 | 9.613  | 13.165 | 13.656 | 1.00 | 17.63 |
| ATOM | 1501 | CB  | PHE | A | 204 | 8.780  | 13.662 | 12.478 | 1.00 | 17.15 |
| ATOM | 1502 | CG  | PHE | A | 204 | 8.211  | 12.569 | 11.663 | 1.00 | 19.02 |
| ATOM | 1503 | CD1 | PHE | A | 204 | 6.914  | 12.146 | 11.891 | 1.00 | 17.04 |
| ATOM | 1504 | CE1 | PHE | A | 204 | 6.350  | 11.116 | 11.141 | 1.00 | 18.50 |
| ATOM | 1505 | CZ  | PHE | A | 204 | 7.075  | 10.508 | 10.152 | 1.00 | 21.34 |
| ATOM | 1506 | CE2 | PHE | A | 204 | 8.386  | 10.932 | 9.889  | 1.00 | 22.09 |
| ATOM | 1507 | CD2 | PHE | A | 204 | 8.952  | 11.967 | 10.652 | 1.00 | 20.96 |

**FIGURE 281**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1508 | C   | PHE | A | 204 | 10.142 | 14.333 | 14.466 | 1.00 | 18.46 |
| ATOM | 1509 | O   | PHE | A | 204 | 9.382  | 15.198 | 14.850 | 1.00 | 19.13 |
| ATOM | 1510 | N   | HIS | A | 205 | 11.448 | 14.343 | 14.733 | 1.00 | 19.90 |
| ATOM | 1511 | CA  | HIS | A | 205 | 12.021 | 15.321 | 15.644 | 1.00 | 19.54 |
| ATOM | 1512 | CB  | HIS | A | 205 | 12.825 | 14.610 | 16.716 | 1.00 | 21.35 |
| ATOM | 1513 | CG  | HIS | A | 205 | 13.401 | 15.519 | 17.747 | 1.00 | 19.20 |
| ATOM | 1514 | ND1 | HIS | A | 205 | 14.407 | 15.127 | 18.610 | 1.00 | 24.56 |
| ATOM | 1515 | CE1 | HIS | A | 205 | 14.724 | 16.142 | 19.394 | 1.00 | 21.30 |
| ATOM | 1516 | NE2 | HIS | A | 205 | 13.962 | 17.173 | 19.071 | 1.00 | 21.10 |
| ATOM | 1517 | CD2 | HIS | A | 205 | 13.130 | 16.813 | 18.036 | 1.00 | 19.44 |
| ATOM | 1518 | C   | HIS | A | 205 | 12.960 | 16.220 | 14.846 | 1.00 | 19.88 |
| ATOM | 1519 | O   | HIS | A | 205 | 14.049 | 15.775 | 14.443 | 1.00 | 18.91 |
| ATOM | 1520 | N   | TYR | A | 206 | 12.504 | 17.456 | 14.670 | 1.00 | 18.79 |
| ATOM | 1521 | CA  | TYR | A | 206 | 13.205 | 18.483 | 13.897 | 1.00 | 18.49 |
| ATOM | 1522 | CB  | TYR | A | 206 | 12.172 | 19.409 | 13.287 | 1.00 | 19.17 |
| ATOM | 1523 | CG  | TYR | A | 206 | 12.754 | 20.435 | 12.354 | 1.00 | 19.28 |
| ATOM | 1524 | CD1 | TYR | A | 206 | 13.004 | 20.115 | 11.023 | 1.00 | 16.50 |
| ATOM | 1525 | CE1 | TYR | A | 206 | 13.540 | 21.052 | 10.141 | 1.00 | 17.88 |
| ATOM | 1526 | CZ  | TYR | A | 206 | 13.831 | 22.327 | 10.588 | 1.00 | 22.43 |
| ATOM | 1527 | OH  | TYR | A | 206 | 14.365 | 23.270 | 9.715  | 1.00 | 25.31 |
| ATOM | 1528 | CE2 | TYR | A | 206 | 13.594 | 22.666 | 11.904 | 1.00 | 23.08 |
| ATOM | 1529 | CD2 | TYR | A | 206 | 13.061 | 21.711 | 12.794 | 1.00 | 23.33 |
| ATOM | 1530 | C   | TYR | A | 206 | 14.064 | 19.229 | 14.900 | 1.00 | 20.26 |
| ATOM | 1531 | O   | TYR | A | 206 | 13.578 | 19.732 | 15.911 | 1.00 | 19.79 |
| ATOM | 1532 | N   | THR | A | 207 | 15.368 | 19.199 | 14.661 | 1.00 | 21.64 |
| ATOM | 1533 | CA  | THR | A | 207 | 16.318 | 19.479 | 15.717 | 1.00 | 23.75 |
| ATOM | 1534 | CB  | THR | A | 207 | 17.403 | 18.361 | 15.771 | 1.00 | 23.14 |
| ATOM | 1535 | OG1 | THR | A | 207 | 17.900 | 18.102 | 14.449 | 1.00 | 24.97 |
| ATOM | 1536 | CG2 | THR | A | 207 | 16.813 | 17.010 | 16.198 | 1.00 | 25.49 |
| ATOM | 1537 | C   | THR | A | 207 | 17.005 | 20.826 | 15.501 | 1.00 | 24.68 |
| ATOM | 1538 | O   | THR | A | 207 | 17.894 | 21.182 | 16.291 | 1.00 | 26.32 |
| ATOM | 1539 | N   | VAL | A | 208 | 16.588 | 21.554 | 14.473 | 1.00 | 24.44 |
| ATOM | 1540 | CA  | VAL | A | 208 | 17.279 | 22.769 | 14.010 | 1.00 | 26.67 |
| ATOM | 1541 | CB  | VAL | A | 208 | 17.996 | 22.597 | 12.627 | 1.00 | 24.93 |
| ATOM | 1542 | CG1 | VAL | A | 208 | 19.123 | 21.595 | 12.712 | 1.00 | 27.87 |
| ATOM | 1543 | CG2 | VAL | A | 208 | 17.022 | 22.243 | 11.490 | 1.00 | 27.01 |
| ATOM | 1544 | C   | VAL | A | 208 | 16.420 | 24.039 | 14.032 | 1.00 | 26.34 |
| ATOM | 1545 | O   | VAL | A | 208 | 16.647 | 24.972 | 13.252 | 1.00 | 29.43 |
| ATOM | 1546 | N   | TRP | A | 209 | 15.419 | 24.083 | 14.903 | 1.00 | 25.54 |
| ATOM | 1547 | CA  | TRP | A | 209 | 14.534 | 25.244 | 14.967 | 1.00 | 24.37 |
| ATOM | 1548 | CB  | TRP | A | 209 | 13.080 | 24.768 | 14.863 | 1.00 | 25.75 |
| ATOM | 1549 | CG  | TRP | A | 209 | 12.082 | 25.820 | 14.491 | 1.00 | 19.87 |
| ATOM | 1550 | CD1 | TRP | A | 209 | 12.153 | 27.174 | 14.694 | 1.00 | 22.45 |
| ATOM | 1551 | NE1 | TRP | A | 209 | 11.034 | 27.786 | 14.183 | 1.00 | 19.81 |
| ATOM | 1552 | CE2 | TRP | A | 209 | 10.202 | 26.822 | 13.663 | 1.00 | 25.00 |
| ATOM | 1553 | CD2 | TRP | A | 209 | 10.834 | 25.575 | 13.847 | 1.00 | 22.65 |
| ATOM | 1554 | CE3 | TRP | A | 209 | 10.185 | 24.414 | 13.399 | 1.00 | 23.01 |
| ATOM | 1555 | CZ3 | TRP | A | 209 | 8.951  | 24.531 | 12.793 | 1.00 | 19.01 |
| ATOM | 1556 | CH2 | TRP | A | 209 | 8.354  | 25.789 | 12.609 | 1.00 | 24.83 |
| ATOM | 1557 | CZ2 | TRP | A | 209 | 8.950  | 26.940 | 13.068 | 1.00 | 22.36 |
| ATOM | 1558 | C   | TRP | A | 209 | 14.678 | 26.021 | 16.270 | 1.00 | 27.04 |
| ATOM | 1559 | O   | TRP | A | 209 | 14.201 | 25.567 | 17.313 | 1.00 | 25.79 |

**FIGURE 282**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1560 | N   | PRO | A | 210 | 15.303 | 27.198 | 16.230 | 1.00 | 28.07 |
| ATOM | 1561 | CA  | PRO | A | 210 | 15.452 | 28.000 | 17.454 | 1.00 | 28.03 |
| ATOM | 1562 | CB  | PRO | A | 210 | 16.386 | 29.140 | 17.022 | 1.00 | 29.50 |
| ATOM | 1563 | CG  | PRO | A | 210 | 16.944 | 28.740 | 15.657 | 1.00 | 31.17 |
| ATOM | 1564 | CD  | PRO | A | 210 | 15.880 | 27.869 | 15.050 | 1.00 | 27.52 |
| ATOM | 1565 | C   | PRO | A | 210 | 14.111 | 28.519 | 17.998 | 1.00 | 28.48 |
| ATOM | 1566 | O   | PRO | A | 210 | 13.268 | 28.944 | 17.216 | 1.00 | 28.98 |
| ATOM | 1567 | N   | ASP | A | 211 | 13.932 | 28.464 | 19.319 | 1.00 | 28.19 |
| ATOM | 1568 | CA  | ASP | A | 211 | 12.736 | 28.971 | 19.993 | 1.00 | 26.86 |
| ATOM | 1569 | CB  | ASP | A | 211 | 12.808 | 28.792 | 21.508 | 1.00 | 27.24 |
| ATOM | 1570 | CG  | ASP | A | 211 | 11.451 | 28.935 | 22.177 | 1.00 | 26.06 |
| ATOM | 1571 | OD1 | ASP | A | 211 | 10.461 | 29.156 | 21.452 | 1.00 | 26.31 |
| ATOM | 1572 | OD2 | ASP | A | 211 | 11.288 | 28.849 | 23.413 | 1.00 | 29.60 |
| ATOM | 1573 | C   | ASP | A | 211 | 12.585 | 30.448 | 19.661 | 1.00 | 28.25 |
| ATOM | 1574 | O   | ASP | A | 211 | 13.577 | 31.180 | 19.556 | 1.00 | 26.45 |
| ATOM | 1575 | N   | HIS | A | 212 | 11.348 | 30.872 | 19.435 | 1.00 | 25.98 |
| ATOM | 1576 | CA  | HIS | A | 212 | 11.107 | 32.260 | 19.072 | 1.00 | 28.34 |
| ATOM | 1577 | CB  | HIS | A | 212 | 11.743 | 33.153 | 20.145 | 1.00 | 29.66 |
| ATOM | 1578 | CG  | HIS | A | 212 | 11.094 | 34.492 | 20.283 | 1.00 | 36.64 |
| ATOM | 1579 | ND1 | HIS | A | 212 | 9.878  | 34.669 | 20.908 | 1.00 | 42.47 |
| ATOM | 1580 | CE1 | HIS | A | 212 | 9.553  | 35.951 | 20.875 | 1.00 | 42.76 |
| ATOM | 1581 | NE2 | HIS | A | 212 | 10.521 | 36.612 | 20.265 | 1.00 | 42.04 |
| ATOM | 1582 | CD2 | HIS | A | 212 | 11.501 | 35.724 | 19.892 | 1.00 | 41.28 |
| ATOM | 1583 | C   | HIS | A | 212 | 11.611 | 32.640 | 17.680 | 1.00 | 28.91 |
| ATOM | 1584 | O   | HIS | A | 212 | 11.494 | 33.799 | 17.275 | 1.00 | 30.92 |
| ATOM | 1585 | N   | GLY | A | 213 | 12.144 | 31.676 | 16.936 | 1.00 | 27.80 |
| ATOM | 1586 | CA  | GLY | A | 213 | 12.751 | 31.971 | 15.650 | 1.00 | 25.99 |
| ATOM | 1587 | C   | GLY | A | 213 | 12.192 | 31.153 | 14.511 | 1.00 | 26.04 |
| ATOM | 1588 | O   | GLY | A | 213 | 11.068 | 30.640 | 14.565 | 1.00 | 24.20 |
| ATOM | 1589 | N   | VAL | A | 214 | 13.012 | 31.066 | 13.470 | 1.00 | 26.25 |
| ATOM | 1590 | CA  | VAL | A | 214 | 12.724 | 30.274 | 12.296 | 1.00 | 26.25 |
| ATOM | 1591 | CB  | VAL | A | 214 | 12.213 | 31.170 | 11.158 | 1.00 | 27.10 |
| ATOM | 1592 | CG1 | VAL | A | 214 | 11.042 | 32.016 | 11.659 | 1.00 | 27.24 |
| ATOM | 1593 | CG2 | VAL | A | 214 | 13.347 | 32.040 | 10.628 | 1.00 | 28.86 |
| ATOM | 1594 | C   | VAL | A | 214 | 13.949 | 29.498 | 11.855 | 1.00 | 24.52 |
| ATOM | 1595 | O   | VAL | A | 214 | 15.095 | 29.866 | 12.167 | 1.00 | 24.97 |
| ATOM | 1596 | N   | PRO | A | 215 | 13.711 | 28.392 | 11.152 | 1.00 | 25.64 |
| ATOM | 1597 | CA  | PRO | A | 215 | 14.793 | 27.622 | 10.526 | 1.00 | 25.48 |
| ATOM | 1598 | CB  | PRO | A | 215 | 14.042 | 26.573 | 9.706  | 1.00 | 26.92 |
| ATOM | 1599 | CG  | PRO | A | 215 | 12.732 | 26.418 | 10.434 | 1.00 | 26.03 |
| ATOM | 1600 | CD  | PRO | A | 215 | 12.380 | 27.805 | 10.901 | 1.00 | 24.12 |
| ATOM | 1601 | C   | PRO | A | 215 | 15.609 | 28.518 | 9.612  | 1.00 | 27.43 |
| ATOM | 1602 | O   | PRO | A | 215 | 15.121 | 29.554 | 9.158  | 1.00 | 27.22 |
| ATOM | 1603 | N   | GLU | A | 216 | 16.841 | 28.111 | 9.315  | 1.00 | 28.05 |
| ATOM | 1604 | CA  | GLU | A | 216 | 17.721 | 28.985 | 8.553  | 1.00 | 28.65 |
| ATOM | 1605 | CB  | GLU | A | 216 | 19.161 | 28.486 | 8.661  | 1.00 | 30.42 |
| ATOM | 1606 | CG  | GLU | A | 216 | 19.771 | 28.747 | 10.023 | 1.00 | 35.56 |
| ATOM | 1607 | CD  | GLU | A | 216 | 21.219 | 29.169 | 9.904  | 1.00 | 42.95 |
| ATOM | 1608 | OE1 | GLU | A | 216 | 21.795 | 28.954 | 8.814  | 1.00 | 48.84 |
| ATOM | 1609 | OE2 | GLU | A | 216 | 21.765 | 29.715 | 10.889 | 1.00 | 45.41 |
| ATOM | 1610 | C   | GLU | A | 216 | 17.315 | 29.114 | 7.087  | 1.00 | 27.95 |
| ATOM | 1611 | O   | GLU | A | 216 | 17.649 | 30.113 | 6.448  | 1.00 | 27.93 |

FIGURE 283

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |       |      |       |
|------|------|-----|-----|---|-----|--------|--------|-------|------|-------|
| ATOM | 1612 | N   | THR | A | 217 | 16.652 | 28.099 | 6.537 | 1.00 | 25.57 |
| ATOM | 1613 | CA  | THR | A | 217 | 16.183 | 28.168 | 5.158 | 1.00 | 24.50 |
| ATOM | 1614 | CB  | THR | A | 217 | 16.913 | 27.146 | 4.270 | 1.00 | 23.44 |
| ATOM | 1615 | OG1 | THR | A | 217 | 16.712 | 25.831 | 4.821 | 1.00 | 23.33 |
| ATOM | 1616 | CG2 | THR | A | 217 | 18.430 | 27.370 | 4.323 | 1.00 | 25.77 |
| ATOM | 1617 | C   | THR | A | 217 | 14.697 | 27.816 | 5.082 | 1.00 | 22.97 |
| ATOM | 1618 | O   | THR | A | 217 | 14.161 | 27.138 | 5.964 | 1.00 | 23.20 |
| ATOM | 1619 | N   | THR | A | 218 | 14.037 | 28.246 | 4.013 | 1.00 | 22.43 |
| ATOM | 1620 | CA  | THR | A | 218 | 12.685 | 27.753 | 3.753 | 1.00 | 21.86 |
| ATOM | 1621 | CB  | THR | A | 218 | 12.003 | 28.563 | 2.637 | 1.00 | 22.40 |
| ATOM | 1622 | OG1 | THR | A | 218 | 12.807 | 28.503 | 1.448 | 1.00 | 23.58 |
| ATOM | 1623 | CG2 | THR | A | 218 | 11.911 | 30.047 | 3.006 | 1.00 | 25.57 |
| ATOM | 1624 | C   | THR | A | 218 | 12.759 | 26.291 | 3.315 | 1.00 | 21.64 |
| ATOM | 1625 | O   | THR | A | 218 | 11.897 | 25.483 | 3.667 | 1.00 | 21.31 |
| ATOM | 1626 | N   | GLN | A | 219 | 13.802 | 25.938 | 2.562 | 1.00 | 21.89 |
| ATOM | 1627 | CA  | GLN | A | 219 | 13.850 | 24.607 | 1.967 | 1.00 | 22.98 |
| ATOM | 1628 | CB  | GLN | A | 219 | 15.019 | 24.424 | 0.995 | 1.00 | 25.47 |
| ATOM | 1629 | CG  | GLN | A | 219 | 16.336 | 23.998 | 1.575 | 1.00 | 35.80 |
| ATOM | 1630 | CD  | GLN | A | 219 | 16.446 | 22.483 | 1.671 | 1.00 | 42.19 |
| ATOM | 1631 | OE1 | GLN | A | 219 | 17.144 | 21.962 | 2.541 | 1.00 | 48.46 |
| ATOM | 1632 | NE2 | GLN | A | 219 | 15.751 | 21.777 | 0.785 | 1.00 | 48.31 |
| ATOM | 1633 | C   | GLN | A | 219 | 13.831 | 23.550 | 3.060 | 1.00 | 22.41 |
| ATOM | 1634 | O   | GLN | A | 219 | 13.184 | 22.523 | 2.872 | 1.00 | 21.59 |
| ATOM | 1635 | N   | SER | A | 220 | 14.509 | 23.809 | 4.180 | 1.00 | 22.02 |
| ATOM | 1636 | CA  | SER | A | 220 | 14.554 | 22.828 | 5.260 | 1.00 | 21.83 |
| ATOM | 1637 | CB  | SER | A | 220 | 15.367 | 23.348 | 6.442 | 1.00 | 24.24 |
| ATOM | 1638 | OG  | SER | A | 220 | 15.366 | 22.396 | 7.489 | 1.00 | 28.06 |
| ATOM | 1639 | C   | SER | A | 220 | 13.157 | 22.477 | 5.785 | 1.00 | 21.60 |
| ATOM | 1640 | O   | SER | A | 220 | 12.768 | 21.309 | 5.802 | 1.00 | 20.80 |
| ATOM | 1641 | N   | LEU | A | 221 | 12.441 | 23.489 | 6.251 | 1.00 | 18.57 |
| ATOM | 1642 | CA  | LEU | A | 221 | 11.111 | 23.186 | 6.787 | 1.00 | 21.03 |
| ATOM | 1643 | CB  | LEU | A | 221 | 10.579 | 24.281 | 7.708 | 1.00 | 22.58 |
| ATOM | 1644 | CG  | LEU | A | 221 | 9.389  | 23.815 | 8.562 | 1.00 | 22.37 |
| ATOM | 1645 | CD1 | LEU | A | 221 | 9.934  | 22.943 | 9.698 | 1.00 | 22.41 |
| ATOM | 1646 | CD2 | LEU | A | 221 | 8.700  | 25.049 | 9.117 | 1.00 | 21.13 |
| ATOM | 1647 | C   | LEU | A | 221 | 10.114 | 22.722 | 5.737 | 1.00 | 21.34 |
| ATOM | 1648 | O   | LEU | A | 221 | 9.317  | 21.822 | 6.010 | 1.00 | 19.35 |
| ATOM | 1649 | N   | ILE | A | 222 | 10.165 | 23.274 | 4.524 | 1.00 | 17.11 |
| ATOM | 1650 | CA  | ILE | A | 222 | 9.335  | 22.740 | 3.456 | 1.00 | 17.94 |
| ATOM | 1651 | CB  | ILE | A | 222 | 9.569  | 23.524 | 2.130 | 1.00 | 17.12 |
| ATOM | 1652 | CG1 | ILE | A | 222 | 9.065  | 24.974 | 2.276 | 1.00 | 19.50 |
| ATOM | 1653 | CD1 | ILE | A | 222 | 9.548  | 25.933 | 1.171 | 1.00 | 19.49 |
| ATOM | 1654 | CG2 | ILE | A | 222 | 8.921  | 22.783 | 0.968 | 1.00 | 21.07 |
| ATOM | 1655 | C   | ILE | A | 222 | 9.601  | 21.260 | 3.217 | 1.00 | 19.20 |
| ATOM | 1656 | O   | ILE | A | 222 | 8.673  | 20.485 | 3.025 | 1.00 | 19.95 |
| ATOM | 1657 | N   | GLN | A | 223 | 10.869 | 20.854 | 3.207 | 1.00 | 16.23 |
| ATOM | 1658 | CA  | GLN | A | 223 | 11.123 | 19.449 | 2.988 | 1.00 | 18.60 |
| ATOM | 1659 | CB  | GLN | A | 223 | 12.616 | 19.228 | 2.715 | 1.00 | 19.15 |
| ATOM | 1660 | CG  | GLN | A | 223 | 12.941 | 17.766 | 2.467 | 1.00 | 22.79 |
| ATOM | 1661 | CD  | GLN | A | 223 | 12.643 | 17.290 | 1.061 | 1.00 | 33.15 |
| ATOM | 1662 | OE1 | GLN | A | 223 | 12.155 | 18.051 | 0.211 | 1.00 | 33.66 |
| ATOM | 1663 | NE2 | GLN | A | 223 | 12.917 | 16.006 | 0.817 | 1.00 | 35.76 |

**FIGURE 284**



|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1664 | C   | GLN | A | 223 | 10.657 | 18.623 | 4.188  | 1.00 | 16.93 |
| ATOM | 1665 | O   | GLN | A | 223 | 10.199 | 17.502 | 3.988  | 1.00 | 18.36 |
| ATOM | 1666 | N   | PHE | A | 224 | 10.797 | 19.161 | 5.401  | 1.00 | 15.46 |
| ATOM | 1667 | CA  | PHE | A | 224 | 10.363 | 18.423 | 6.587  | 1.00 | 15.62 |
| ATOM | 1668 | CB  | PHE | A | 224 | 10.706 | 19.198 | 7.848  | 1.00 | 17.10 |
| ATOM | 1669 | CG  | PHE | A | 224 | 10.337 | 18.487 | 9.120  | 1.00 | 16.49 |
| ATOM | 1670 | CD1 | PHE | A | 224 | 10.836 | 17.215 | 9.398  | 1.00 | 17.51 |
| ATOM | 1671 | CE1 | PHE | A | 224 | 10.531 | 16.576 | 10.616 | 1.00 | 17.07 |
| ATOM | 1672 | CZ  | PHE | A | 224 | 9.717  | 17.205 | 11.544 | 1.00 | 16.55 |
| ATOM | 1673 | CE2 | PHE | A | 224 | 9.212  | 18.492 | 11.279 | 1.00 | 18.07 |
| ATOM | 1674 | CD2 | PHE | A | 224 | 9.544  | 19.125 | 10.054 | 1.00 | 19.46 |
| ATOM | 1675 | C   | PHE | A | 224 | 8.855  | 18.199 | 6.531  | 1.00 | 16.89 |
| ATOM | 1676 | O   | PHE | A | 224 | 8.380  | 17.078 | 6.751  | 1.00 | 16.66 |
| ATOM | 1677 | N   | VAL | A | 225 | 8.122  | 19.270 | 6.265  | 1.00 | 17.58 |
| ATOM | 1678 | CA  | VAL | A | 225 | 6.654  | 19.197 | 6.213  | 1.00 | 18.48 |
| ATOM | 1679 | CB  | VAL | A | 225 | 6.084  | 20.603 | 5.951  | 1.00 | 19.47 |
| ATOM | 1680 | CG1 | VAL | A | 225 | 4.635  | 20.522 | 5.473  | 1.00 | 20.27 |
| ATOM | 1681 | CG2 | VAL | A | 225 | 6.211  | 21.475 | 7.199  | 1.00 | 17.11 |
| ATOM | 1682 | C   | VAL | A | 225 | 6.241  | 18.203 | 5.122  | 1.00 | 19.13 |
| ATOM | 1683 | O   | VAL | A | 225 | 5.402  | 17.311 | 5.312  | 1.00 | 21.63 |
| ATOM | 1684 | N   | ARG | A | 226 | 6.829  | 18.331 | 3.941  | 1.00 | 19.30 |
| ATOM | 1685 | CA  | ARG | A | 226 | 6.514  | 17.393 | 2.871  | 1.00 | 20.41 |
| ATOM | 1686 | CB  | ARG | A | 226 | 7.276  | 17.776 | 1.594  | 1.00 | 20.66 |
| ATOM | 1687 | CG  | ARG | A | 226 | 6.656  | 18.990 | 0.916  | 1.00 | 22.30 |
| ATOM | 1688 | CD  | ARG | A | 226 | 7.410  | 19.483 | -0.302 | 1.00 | 24.61 |
| ATOM | 1689 | NE  | ARG | A | 226 | 6.694  | 20.558 | -0.983 | 1.00 | 24.83 |
| ATOM | 1690 | CZ  | ARG | A | 226 | 7.223  | 21.308 | -1.948 | 1.00 | 31.14 |
| ATOM | 1691 | NH1 | ARG | A | 226 | 8.489  | 21.146 | -2.306 | 1.00 | 30.48 |
| ATOM | 1692 | NH2 | ARG | A | 226 | 6.500  | 22.253 | -2.526 | 1.00 | 34.90 |
| ATOM | 1693 | C   | ARG | A | 226 | 6.797  | 15.932 | 3.234  | 1.00 | 20.34 |
| ATOM | 1694 | O   | ARG | A | 226 | 6.060  | 15.004 | 2.879  | 1.00 | 19.67 |
| ATOM | 1695 | N   | THR | A | 227 | 7.910  | 15.717 | 3.920  | 1.00 | 19.65 |
| ATOM | 1696 | CA  | THR | A | 227 | 8.323  | 14.388 | 4.338  | 1.00 | 20.52 |
| ATOM | 1697 | CB  | THR | A | 227 | 9.715  | 14.485 | 4.977  | 1.00 | 22.22 |
| ATOM | 1698 | OG1 | THR | A | 227 | 10.673 | 14.679 | 3.930  | 1.00 | 22.33 |
| ATOM | 1699 | CG2 | THR | A | 227 | 10.110 | 13.143 | 5.586  | 1.00 | 24.52 |
| ATOM | 1700 | C   | THR | A | 227 | 7.310  | 13.786 | 5.339  | 1.00 | 20.30 |
| ATOM | 1701 | O   | THR | A | 227 | 6.886  | 12.642 | 5.191  | 1.00 | 20.93 |
| ATOM | 1702 | N   | VAL | A | 228 | 6.918  | 14.576 | 6.335  | 1.00 | 19.24 |
| ATOM | 1703 | CA  | VAL | A | 228 | 5.954  | 14.152 | 7.348  | 1.00 | 19.59 |
| ATOM | 1704 | CB  | VAL | A | 228 | 5.778  | 15.216 | 8.430  | 1.00 | 19.58 |
| ATOM | 1705 | CG1 | VAL | A | 228 | 4.631  | 14.832 | 9.353  | 1.00 | 20.61 |
| ATOM | 1706 | CG2 | VAL | A | 228 | 7.077  | 15.408 | 9.206  | 1.00 | 19.73 |
| ATOM | 1707 | C   | VAL | A | 228 | 4.609  | 13.877 | 6.690  | 1.00 | 21.77 |
| ATOM | 1708 | O   | VAL | A | 228 | 4.013  | 12.844 | 6.938  | 1.00 | 21.18 |
| ATOM | 1709 | N   | ARG | A | 229 | 4.183  | 14.774 | 5.805  | 1.00 | 22.98 |
| ATOM | 1710 | CA  | ARG | A | 229 | 2.866  | 14.626 | 5.179  | 1.00 | 25.81 |
| ATOM | 1711 | CB  | ARG | A | 229 | 2.546  | 15.904 | 4.402  | 1.00 | 23.29 |
| ATOM | 1712 | CG  | ARG | A | 229 | 1.423  | 15.881 | 3.384  | 1.00 | 28.30 |
| ATOM | 1713 | CD  | ARG | A | 229 | 0.053  | 15.877 | 3.972  | 1.00 | 30.57 |
| ATOM | 1714 | NE  | ARG | A | 229 | -0.051 | 16.615 | 5.222  | 1.00 | 30.38 |
| ATOM | 1715 | CZ  | ARG | A | 229 | -0.925 | 16.290 | 6.160  | 1.00 | 29.65 |

**FIGURE 285**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |       |      |       |
|------|------|-----|-----|---|-----|--------|--------|-------|------|-------|
| ATOM | 1716 | NH1 | ARG | A | 229 | -1.763 | 15.279 | 5.941 | 1.00 | 32.05 |
| ATOM | 1717 | NH2 | ARG | A | 229 | -0.987 | 16.980 | 7.291 | 1.00 | 29.06 |
| ATOM | 1718 | C   | ARG | A | 229 | 2.879  | 13.378 | 4.301 | 1.00 | 26.73 |
| ATOM | 1719 | O   | ARG | A | 229 | 1.879  | 12.653 | 4.242 | 1.00 | 27.86 |
| ATOM | 1720 | N   | ASP | A | 230 | 4.015  | 13.108 | 3.658 | 1.00 | 26.22 |
| ATOM | 1721 | CA  | ASP | A | 230 | 4.251  | 11.866 | 2.928 | 1.00 | 28.24 |
| ATOM | 1722 | CB  | ASP | A | 230 | 5.621  | 11.877 | 2.251 | 1.00 | 28.67 |
| ATOM | 1723 | CG  | ASP | A | 230 | 5.654  | 12.720 | 0.982 | 1.00 | 34.01 |
| ATOM | 1724 | OD1 | ASP | A | 230 | 4.609  | 13.162 | 0.469 | 1.00 | 39.53 |
| ATOM | 1725 | OD2 | ASP | A | 230 | 6.727  | 13.005 | 0.420 | 1.00 | 41.90 |
| ATOM | 1726 | C   | ASP | A | 230 | 4.071  | 10.598 | 3.770 | 1.00 | 29.04 |
| ATOM | 1727 | O   | ASP | A | 230 | 3.401  | 9.645  | 3.350 | 1.00 | 29.94 |
| ATOM | 1728 | N   | TYR | A | 231 | 4.625  | 10.592 | 4.979 | 1.00 | 25.95 |
| ATOM | 1729 | CA  | TYR | A | 231 | 4.433  | 9.452  | 5.871 | 1.00 | 26.50 |
| ATOM | 1730 | CB  | TYR | A | 231 | 5.319  | 9.550  | 7.113 | 1.00 | 26.14 |
| ATOM | 1731 | CG  | TYR | A | 231 | 6.748  | 9.078  | 6.927 | 1.00 | 23.97 |
| ATOM | 1732 | CD1 | TYR | A | 231 | 7.774  | 9.978  | 6.647 | 1.00 | 19.78 |
| ATOM | 1733 | CE1 | TYR | A | 231 | 9.081  | 9.547  | 6.522 | 1.00 | 22.19 |
| ATOM | 1734 | CZ  | TYR | A | 231 | 9.390  | 8.211  | 6.654 | 1.00 | 23.00 |
| ATOM | 1735 | OH  | TYR | A | 231 | 10.701 | 7.787  | 6.513 | 1.00 | 28.03 |
| ATOM | 1736 | CE2 | TYR | A | 231 | 8.401  | 7.304  | 6.947 | 1.00 | 27.25 |
| ATOM | 1737 | CD2 | TYR | A | 231 | 7.086  | 7.736  | 7.088 | 1.00 | 25.16 |
| ATOM | 1738 | C   | TYR | A | 231 | 2.970  | 9.323  | 6.291 | 1.00 | 27.31 |
| ATOM | 1739 | O   | TYR | A | 231 | 2.446  | 8.209  | 6.297 | 1.00 | 28.55 |
| ATOM | 1740 | N   | ILE | A | 232 | 2.347  | 10.443 | 6.652 | 1.00 | 26.87 |
| ATOM | 1741 | CA  | ILE | A | 232 | 0.914  | 10.502 | 6.996 | 1.00 | 27.98 |
| ATOM | 1742 | CB  | ILE | A | 232 | 0.491  | 11.959 | 7.360 | 1.00 | 25.62 |
| ATOM | 1743 | CG1 | ILE | A | 232 | 1.038  | 12.361 | 8.727 | 1.00 | 26.35 |
| ATOM | 1744 | CD1 | ILE | A | 232 | 0.938  | 13.838 | 8.996 | 1.00 | 27.73 |
| ATOM | 1745 | CG2 | ILE | A | 232 | -1.058 | 12.159 | 7.424 | 1.00 | 25.67 |
| ATOM | 1746 | C   | ILE | A | 232 | 0.046  | 9.935  | 5.875 | 1.00 | 32.06 |
| ATOM | 1747 | O   | ILE | A | 232 | -0.767 | 9.022  | 6.107 | 1.00 | 33.57 |
| ATOM | 1748 | N   | ASN | A | 233 | 0.245  | 10.451 | 4.663 | 1.00 | 33.34 |
| ATOM | 1749 | CA  | ASN | A | 233 | -0.580 | 10.101 | 3.509 | 1.00 | 37.27 |
| ATOM | 1750 | CB  | ASN | A | 233 | -0.320 | 11.037 | 2.313 | 1.00 | 36.54 |
| ATOM | 1751 | CG  | ASN | A | 233 | -0.932 | 12.425 | 2.480 | 1.00 | 38.15 |
| ATOM | 1752 | OD1 | ASN | A | 233 | -1.648 | 12.712 | 3.442 | 1.00 | 42.42 |
| ATOM | 1753 | ND2 | ASN | A | 233 | -0.630 | 13.309 | 1.533 | 1.00 | 37.50 |
| ATOM | 1754 | C   | ASN | A | 233 | -0.429 | 8.635  | 3.090 | 1.00 | 39.12 |
| ATOM | 1755 | O   | ASN | A | 233 | -1.332 | 8.073  | 2.463 | 1.00 | 41.73 |
| ATOM | 1756 | N   | ARG | A | 234 | 0.690  | 8.001  | 3.431 | 1.00 | 40.44 |
| ATOM | 1757 | CA  | ARG | A | 234 | 0.962  | 6.653  | 2.945 | 1.00 | 42.23 |
| ATOM | 1758 | CB  | ARG | A | 234 | 2.455  | 6.462  | 2.658 | 1.00 | 43.61 |
| ATOM | 1759 | CG  | ARG | A | 234 | 2.949  | 7.205  | 1.408 | 1.00 | 43.04 |
| ATOM | 1760 | CD  | ARG | A | 234 | 4.330  | 6.793  | 0.906 | 1.00 | 48.69 |
| ATOM | 1761 | NE  | ARG | A | 234 | 5.341  | 6.796  | 1.963 | 1.00 | 51.23 |
| ATOM | 1762 | CZ  | ARG | A | 234 | 6.283  | 7.724  | 2.115 | 1.00 | 54.19 |
| ATOM | 1763 | NH1 | ARG | A | 234 | 6.365  | 8.748  | 1.272 | 1.00 | 52.70 |
| ATOM | 1764 | NH2 | ARG | A | 234 | 7.144  | 7.630  | 3.122 | 1.00 | 51.22 |
| ATOM | 1765 | C   | ARG | A | 234 | 0.400  | 5.566  | 3.863 | 1.00 | 42.06 |
| ATOM | 1766 | O   | ARG | A | 234 | 0.337  | 4.379  | 3.512 | 1.00 | 42.43 |
| ATOM | 1767 | N   | SER | A | 235 | -0.055 | 6.003  | 5.031 | 1.00 | 40.54 |

**FIGURE 286**

|      |      |     |           |        |        |        |      |       |
|------|------|-----|-----------|--------|--------|--------|------|-------|
| ATOM | 1768 | CA  | SER A 235 | -0.488 | 5.108  | 6.087  | 1.00 | 39.57 |
| ATOM | 1769 | CB  | SER A 235 | -0.193 | 5.750  | 7.451  | 1.00 | 39.71 |
| ATOM | 1770 | OG  | SER A 235 | -1.211 | 5.554  | 8.422  | 1.00 | 41.17 |
| ATOM | 1771 | C   | SER A 235 | -1.964 | 4.744  | 5.925  | 1.00 | 38.09 |
| ATOM | 1772 | O   | SER A 235 | -2.799 | 5.592  | 5.590  | 1.00 | 36.22 |
| ATOM | 1773 | N   | PRO A 236 | -2.278 | 3.477  | 6.177  | 1.00 | 38.34 |
| ATOM | 1774 | CA  | PRO A 236 | -3.661 | 2.979  | 6.083  | 1.00 | 39.35 |
| ATOM | 1775 | CB  | PRO A 236 | -3.537 | 1.499  | 6.461  | 1.00 | 40.18 |
| ATOM | 1776 | CG  | PRO A 236 | -2.214 | 1.375  | 7.150  | 1.00 | 39.24 |
| ATOM | 1777 | CD  | PRO A 236 | -1.322 | 2.425  | 6.563  | 1.00 | 38.58 |
| ATOM | 1778 | C   | PRO A 236 | -4.678 | 3.691  | 6.987  | 1.00 | 39.63 |
| ATOM | 1779 | O   | PRO A 236 | -5.889 | 3.488  | 6.852  | 1.00 | 42.61 |
| ATOM | 1780 | N   | GLY A 237 | -4.208 | 4.544  | 7.889  | 1.00 | 36.88 |
| ATOM | 1781 | CA  | GLY A 237 | -5.069 | 5.079  | 8.938  | 1.00 | 34.20 |
| ATOM | 1782 | C   | GLY A 237 | -4.178 | 5.738  | 9.970  | 1.00 | 30.76 |
| ATOM | 1783 | O   | GLY A 237 | -3.532 | 5.037  | 10.733 | 1.00 | 29.45 |
| ATOM | 1784 | N   | ALA A 238 | -4.150 | 7.071  | 9.986  | 1.00 | 28.97 |
| ATOM | 1785 | CA  | ALA A 238 | -3.119 | 7.844  | 10.698 | 1.00 | 24.56 |
| ATOM | 1786 | CB  | ALA A 238 | -2.656 | 9.019  | 9.834  | 1.00 | 27.03 |
| ATOM | 1787 | C   | ALA A 238 | -3.564 | 8.342  | 12.077 | 1.00 | 23.45 |
| ATOM | 1788 | O   | ALA A 238 | -2.759 | 8.476  | 12.986 | 1.00 | 21.78 |
| ATOM | 1789 | N   | GLY A 239 | -4.853 | 8.620  | 12.242 | 1.00 | 21.70 |
| ATOM | 1790 | CA  | GLY A 239 | -5.342 | 9.313  | 13.423 | 1.00 | 21.30 |
| ATOM | 1791 | C   | GLY A 239 | -4.903 | 10.766 | 13.366 | 1.00 | 19.24 |
| ATOM | 1792 | O   | GLY A 239 | -4.282 | 11.186 | 12.388 | 1.00 | 18.48 |
| ATOM | 1793 | N   | PRO A 240 | -5.233 | 11.526 | 14.405 | 1.00 | 20.05 |
| ATOM | 1794 | CA  | PRO A 240 | -4.740 | 12.907 | 14.530 | 1.00 | 19.68 |
| ATOM | 1795 | CB  | PRO A 240 | -5.327 | 13.390 | 15.861 | 1.00 | 18.80 |
| ATOM | 1796 | CG  | PRO A 240 | -6.393 | 12.393 | 16.247 | 1.00 | 21.11 |
| ATOM | 1797 | CD  | PRO A 240 | -6.041 | 11.103 | 15.562 | 1.00 | 20.23 |
| ATOM | 1798 | C   | PRO A 240 | -3.213 | 12.834 | 14.624 | 1.00 | 18.33 |
| ATOM | 1799 | O   | PRO A 240 | -2.661 | 11.864 | 15.141 | 1.00 | 19.27 |
| ATOM | 1800 | N   | THR A 241 | -2.548 | 13.832 | 14.071 | 1.00 | 16.60 |
| ATOM | 1801 | CA  | THR A 241 | -1.090 | 13.930 | 14.185 | 1.00 | 15.99 |
| ATOM | 1802 | CB  | THR A 241 | -0.593 | 14.614 | 12.919 | 1.00 | 15.63 |
| ATOM | 1803 | OG1 | THR A 241 | -0.797 | 13.696 | 11.849 | 1.00 | 17.20 |
| ATOM | 1804 | CG2 | THR A 241 | 0.941  | 14.788 | 12.984 | 1.00 | 15.00 |
| ATOM | 1805 | C   | THR A 241 | -0.829 | 14.832 | 15.367 | 1.00 | 16.75 |
| ATOM | 1806 | O   | THR A 241 | -1.343 | 15.938 | 15.418 | 1.00 | 17.15 |
| ATOM | 1807 | N   | VAL A 242 | 0.031  | 14.387 | 16.274 | 1.00 | 16.56 |
| ATOM | 1808 | CA  | VAL A 242 | 0.370  | 15.207 | 17.413 | 1.00 | 15.30 |
| ATOM | 1809 | CB  | VAL A 242 | 0.777  | 14.315 | 18.586 | 1.00 | 13.91 |
| ATOM | 1810 | CG1 | VAL A 242 | 1.584  | 15.122 | 19.651 | 1.00 | 17.96 |
| ATOM | 1811 | CG2 | VAL A 242 | -0.473 | 13.828 | 19.205 | 1.00 | 14.74 |
| ATOM | 1812 | C   | VAL A 242 | 1.537  | 16.089 | 17.002 | 1.00 | 15.85 |
| ATOM | 1813 | O   | VAL A 242 | 2.491  | 15.610 | 16.401 | 1.00 | 17.01 |
| ATOM | 1814 | N   | VAL A 243 | 1.421  | 17.375 | 17.295 | 1.00 | 15.52 |
| ATOM | 1815 | CA  | VAL A 243 | 2.525  | 18.289 | 17.027 | 1.00 | 15.21 |
| ATOM | 1816 | CB  | VAL A 243 | 2.223  | 19.311 | 15.915 | 1.00 | 13.92 |
| ATOM | 1817 | CG1 | VAL A 243 | 3.540  | 20.039 | 15.607 | 1.00 | 15.53 |
| ATOM | 1818 | CG2 | VAL A 243 | 1.710  | 18.648 | 14.624 | 1.00 | 15.61 |
| ATOM | 1819 | C   | VAL A 243 | 2.848  | 19.042 | 18.309 | 1.00 | 13.38 |

FIGURE 287

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 1820 | O   | VAL | A | 243 | 1.977  | 19.511 | 19.006 | 1.00 | 15.35 |
| ATOM | 1821 | N   | HIS | A | 244 | 4.127  | 19.115 | 18.681 | 1.00 | 13.84 |
| ATOM | 1822 | CA  | HIS | A | 244 | 4.487  | 19.880 | 19.875 | 1.00 | 13.12 |
| ATOM | 1823 | CB  | HIS | A | 244 | 4.399  | 19.034 | 21.167 | 1.00 | 11.87 |
| ATOM | 1824 | CG  | HIS | A | 244 | 5.560  | 18.115 | 21.377 | 1.00 | 15.41 |
| ATOM | 1825 | ND1 | HIS | A | 244 | 6.728  | 18.524 | 21.977 | 1.00 | 16.81 |
| ATOM | 1826 | CE1 | HIS | A | 244 | 7.566  | 17.503 | 22.042 | 1.00 | 16.27 |
| ATOM | 1827 | NE2 | HIS | A | 244 | 6.998  | 16.461 | 21.463 | 1.00 | 16.52 |
| ATOM | 1828 | CD2 | HIS | A | 244 | 5.726  | 16.808 | 21.067 | 1.00 | 14.38 |
| ATOM | 1829 | C   | HIS | A | 244 | 5.856  | 20.526 | 19.735 | 1.00 | 14.17 |
| ATOM | 1830 | O   | HIS | A | 244 | 6.688  | 20.046 | 18.970 | 1.00 | 16.93 |
| ATOM | 1831 | N   | CYS | A | 245 | 6.041  | 21.611 | 20.492 | 1.00 | 16.57 |
| ATOM | 1832 | CA  | CYS | A | 245 | 7.349  | 22.211 | 20.652 | 1.00 | 17.05 |
| ATOM | 1833 | CB  | CYS | A | 245 | 7.396  | 23.573 | 19.941 | 1.00 | 15.83 |
| ATOM | 1834 | SG  | CYS | A | 245 | 5.834  | 24.486 | 20.086 | 1.00 | 19.56 |
| ATOM | 1835 | C   | CYS | A | 245 | 7.521  | 22.283 | 22.151 | 1.00 | 17.57 |
| ATOM | 1836 | O   | CYS | A | 245 | 7.391  | 21.246 | 22.839 | 1.00 | 17.79 |
| ATOM | 1837 | N   | SER | A | 246 | 7.815  | 23.464 | 22.693 | 1.00 | 18.50 |
| ATOM | 1838 | CA  | SER | A | 246 | 7.937  | 23.554 | 24.159 | 1.00 | 16.87 |
| ATOM | 1839 | CB  | SER | A | 246 | 9.020  | 24.552 | 24.628 | 1.00 | 18.69 |
| ATOM | 1840 | OG  | SER | A | 246 | 9.228  | 24.422 | 26.031 | 1.00 | 18.18 |
| ATOM | 1841 | C   | SER | A | 246 | 6.573  | 23.942 | 24.722 | 1.00 | 17.49 |
| ATOM | 1842 | O   | SER | A | 246 | 6.046  | 23.238 | 25.580 | 1.00 | 17.21 |
| ATOM | 1843 | N   | ALA | A | 247 | 6.019  | 25.049 | 24.239 | 1.00 | 18.04 |
| ATOM | 1844 | CA  | ALA | A | 247 | 4.736  | 25.497 | 24.749 | 1.00 | 19.26 |
| ATOM | 1845 | CB  | ALA | A | 247 | 4.710  | 27.036 | 24.838 | 1.00 | 19.87 |
| ATOM | 1846 | C   | ALA | A | 247 | 3.573  | 25.010 | 23.903 | 1.00 | 17.94 |
| ATOM | 1847 | O   | ALA | A | 247 | 2.430  | 25.177 | 24.309 | 1.00 | 19.75 |
| ATOM | 1848 | N   | GLY | A | 248 | 3.848  | 24.439 | 22.729 | 1.00 | 20.22 |
| ATOM | 1849 | CA  | GLY | A | 248 | 2.806  | 24.174 | 21.748 | 1.00 | 18.63 |
| ATOM | 1850 | C   | GLY | A | 248 | 2.132  | 25.433 | 21.196 | 1.00 | 18.85 |
| ATOM | 1851 | O   | GLY | A | 248 | 0.898  | 25.475 | 21.017 | 1.00 | 19.05 |
| ATOM | 1852 | N   | VAL | A | 249 | 2.954  | 26.427 | 20.867 | 1.00 | 17.12 |
| ATOM | 1853 | CA  | VAL | A | 249 | 2.463  | 27.715 | 20.358 | 1.00 | 16.65 |
| ATOM | 1854 | CB  | VAL | A | 249 | 2.562  | 28.810 | 21.445 | 1.00 | 18.34 |
| ATOM | 1855 | CG1 | VAL | A | 249 | 2.075  | 30.142 | 20.845 | 1.00 | 21.79 |
| ATOM | 1856 | CG2 | VAL | A | 249 | 1.744  | 28.426 | 22.662 | 1.00 | 20.69 |
| ATOM | 1857 | C   | VAL | A | 249 | 3.164  | 28.180 | 19.070 | 1.00 | 17.87 |
| ATOM | 1858 | O   | VAL | A | 249 | 2.543  | 28.251 | 18.008 | 1.00 | 17.85 |
| ATOM | 1859 | N   | GLY | A | 250 | 4.453  | 28.487 | 19.140 | 1.00 | 19.22 |
| ATOM | 1860 | CA  | GLY | A | 250 | 5.039  | 29.253 | 18.055 | 1.00 | 19.94 |
| ATOM | 1861 | C   | GLY | A | 250 | 5.491  | 28.321 | 16.963 | 1.00 | 19.70 |
| ATOM | 1862 | O   | GLY | A | 250 | 5.086  | 28.456 | 15.808 | 1.00 | 19.01 |
| ATOM | 1863 | N   | ARG | A | 251 | 6.366  | 27.389 | 17.335 | 1.00 | 19.14 |
| ATOM | 1864 | CA  | ARG | A | 251 | 6.939  | 26.498 | 16.347 | 1.00 | 19.05 |
| ATOM | 1865 | CB  | ARG | A | 251 | 8.195  | 25.860 | 16.890 | 1.00 | 19.24 |
| ATOM | 1866 | CG  | ARG | A | 251 | 9.219  | 26.952 | 17.158 | 1.00 | 15.81 |
| ATOM | 1867 | CD  | ARG | A | 251 | 10.481 | 26.394 | 17.775 | 1.00 | 16.06 |
| ATOM | 1868 | NE  | ARG | A | 251 | 10.226 | 26.200 | 19.214 | 1.00 | 19.50 |
| ATOM | 1869 | CZ  | ARG | A | 251 | 11.094 | 25.704 | 20.078 | 1.00 | 22.30 |
| ATOM | 1870 | NH1 | ARG | A | 251 | 12.290 | 25.314 | 19.644 | 1.00 | 20.21 |
| ATOM | 1871 | NH2 | ARG | A | 251 | 10.758 | 25.569 | 21.366 | 1.00 | 23.16 |

**FIGURE 288**

|      |      |     |      |   |     |        |        |        |      |       |
|------|------|-----|------|---|-----|--------|--------|--------|------|-------|
| ATOM | 1872 | C   | ARG  | A | 251 | 5.901  | 25.497 | 15.876 | 1.00 | 18.56 |
| ATOM | 1873 | O   | ARG  | A | 251 | 5.813  | 25.250 | 14.680 | 1.00 | 17.43 |
| ATOM | 1874 | N   | THR  | A | 252 | 5.111  | 24.941 | 16.794 | 1.00 | 18.19 |
| ATOM | 1875 | CA  | THR  | A | 252 | 3.982  | 24.106 | 16.377 | 1.00 | 17.71 |
| ATOM | 1876 | CB  | THR  | A | 252 | 3.217  | 23.628 | 17.607 | 1.00 | 17.40 |
| ATOM | 1877 | OG1 | ATHR | A | 252 | 2.999  | 24.765 | 18.450 | 0.50 | 23.23 |
| ATOM | 1878 | OG1 | BTHR | A | 252 | 4.029  | 22.684 | 18.306 | 0.50 | 13.92 |
| ATOM | 1879 | CG2 | ATHR | A | 252 | 4.083  | 22.722 | 18.434 | 0.50 | 15.60 |
| ATOM | 1880 | CG2 | BTHR | A | 252 | 1.947  | 22.833 | 17.252 | 0.50 | 10.20 |
| ATOM | 1881 | C   | THR  | A | 252 | 3.019  | 24.851 | 15.484 | 1.00 | 17.17 |
| ATOM | 1882 | O   | THR  | A | 252 | 2.600  | 24.297 | 14.475 | 1.00 | 15.23 |
| ATOM | 1883 | N   | GLY  | A | 253 | 2.661  | 26.092 | 15.832 | 1.00 | 16.60 |
| ATOM | 1884 | CA  | GLY  | A | 253 | 1.745  | 26.853 | 14.990 | 1.00 | 16.77 |
| ATOM | 1885 | C   | GLY  | A | 253 | 2.300  | 27.075 | 13.599 | 1.00 | 17.58 |
| ATOM | 1886 | O   | GLY  | A | 253 | 1.597  | 26.966 | 12.604 | 1.00 | 16.20 |
| ATOM | 1887 | N   | THR  | A | 254 | 3.608  | 27.343 | 13.507 | 1.00 | 15.25 |
| ATOM | 1888 | CA  | THR  | A | 254 | 4.197  | 27.626 | 12.216 | 1.00 | 14.32 |
| ATOM | 1889 | CB  | THR  | A | 254 | 5.628  | 28.249 | 12.422 | 1.00 | 13.48 |
| ATOM | 1890 | OG1 | THR  | A | 254 | 5.439  | 29.443 | 13.202 | 1.00 | 18.67 |
| ATOM | 1891 | CG2 | THR  | A | 254 | 6.190  | 28.764 | 11.050 | 1.00 | 17.19 |
| ATOM | 1892 | C   | THR  | A | 254 | 4.262  | 26.342 | 11.390 | 1.00 | 15.60 |
| ATOM | 1893 | O   | THR  | A | 254 | 4.052  | 26.379 | 10.184 | 1.00 | 17.10 |
| ATOM | 1894 | N   | PHE  | A | 255 | 4.576  | 25.222 | 12.032 | 1.00 | 15.48 |
| ATOM | 1895 | CA  | PHE  | A | 255 | 4.640  | 23.944 | 11.321 | 1.00 | 15.29 |
| ATOM | 1896 | CB  | PHE  | A | 255 | 5.043  | 22.832 | 12.304 | 1.00 | 17.14 |
| ATOM | 1897 | CG  | PHE  | A | 255 | 4.977  | 21.465 | 11.674 | 1.00 | 17.46 |
| ATOM | 1898 | CD1 | PHE  | A | 255 | 6.052  | 21.001 | 10.959 | 1.00 | 20.12 |
| ATOM | 1899 | CE1 | PHE  | A | 255 | 6.001  | 19.759 | 10.330 | 1.00 | 19.80 |
| ATOM | 1900 | CZ  | PHE  | A | 255 | 4.860  | 19.003 | 10.351 | 1.00 | 15.16 |
| ATOM | 1901 | CE2 | PHE  | A | 255 | 3.755  | 19.457 | 11.013 | 1.00 | 16.37 |
| ATOM | 1902 | CD2 | PHE  | A | 255 | 3.796  | 20.725 | 11.662 | 1.00 | 15.77 |
| ATOM | 1903 | C   | PHE  | A | 255 | 3.271  | 23.608 | 10.725 | 1.00 | 15.30 |
| ATOM | 1904 | O   | PHE  | A | 255 | 3.145  | 23.207 | 9.548  | 1.00 | 15.54 |
| ATOM | 1905 | N   | ILE  | A | 256 | 2.256  | 23.693 | 11.568 | 1.00 | 13.96 |
| ATOM | 1906 | CA  | ILE  | A | 256 | 0.914  | 23.321 | 11.106 | 1.00 | 14.62 |
| ATOM | 1907 | CB  | ILE  | A | 256 | -0.077 | 23.288 | 12.256 | 1.00 | 14.78 |
| ATOM | 1908 | CG1 | ILE  | A | 256 | 0.284  | 22.166 | 13.221 | 1.00 | 16.14 |
| ATOM | 1909 | CD1 | ILE  | A | 256 | -0.671 | 22.068 | 14.439 | 1.00 | 16.04 |
| ATOM | 1910 | CG2 | ILE  | A | 256 | -1.497 | 23.016 | 11.695 | 1.00 | 14.89 |
| ATOM | 1911 | C   | ILE  | A | 256 | 0.465  | 24.282 | 9.993  | 1.00 | 14.00 |
| ATOM | 1912 | O   | ILE  | A | 256 | -0.065 | 23.831 | 8.975  | 1.00 | 15.99 |
| ATOM | 1913 | N   | ALA  | A | 257 | 0.637  | 25.588 | 10.195 | 1.00 | 14.29 |
| ATOM | 1914 | CA  | ALA  | A | 257 | 0.292  | 26.539 | 9.130  | 1.00 | 13.84 |
| ATOM | 1915 | CB  | ALA  | A | 257 | 0.571  | 27.988 | 9.530  | 1.00 | 14.99 |
| ATOM | 1916 | C   | ALA  | A | 257 | 0.955  | 26.205 | 7.798  | 1.00 | 14.85 |
| ATOM | 1917 | O   | ALA  | A | 257 | 0.328  | 26.208 | 6.746  | 1.00 | 16.25 |
| ATOM | 1918 | N   | LEU  | A | 258 | 2.258  | 25.958 | 7.833  | 1.00 | 13.44 |
| ATOM | 1919 | CA  | LEU  | A | 258 | 2.950  | 25.564 | 6.631  | 1.00 | 14.78 |
| ATOM | 1920 | CB  | LEU  | A | 258 | 4.448  | 25.390 | 6.889  | 1.00 | 13.66 |
| ATOM | 1921 | CG  | LEU  | A | 258 | 5.247  | 25.137 | 5.615  | 1.00 | 15.58 |
| ATOM | 1922 | CD1 | LEU  | A | 258 | 5.050  | 26.284 | 4.593  | 1.00 | 17.44 |
| ATOM | 1923 | CD2 | LEU  | A | 258 | 6.745  | 25.019 | 5.965  | 1.00 | 16.74 |

**FIGURE 289**

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|      |      |         |     |     |        |        |        |        |       |       |
|------|------|---------|-----|-----|--------|--------|--------|--------|-------|-------|
| ATOM | 1924 | C       | LEU | A   | 258    | 2.391  | 24.297 | 6.013  | 1.00  | 14.93 |
| ATOM | 1925 | O       | LEU | A   | 258    | 2.223  | 24.210 | 4.805  | 1.00  | 14.85 |
| ATOM | 1926 | N       | ASP | A   | 259    | 2.105  | 23.290 | 6.838  | 1.00  | 15.85 |
| ATOM | 1927 | CA      | ASP | A   | 259    | 1.470  | 22.081 | 6.314  | 1.00  | 16.95 |
| ATOM | 1928 | CB      | ASP | A   | 259    | 1.186  | 21.146 | 7.501  | 1.00  | 18.21 |
| ATOM | 1929 | CG      | ASP | A   | 259    | 0.834  | 19.718 | 7.102  | 1.00  | 22.66 |
| ATOM | 1930 | OD1     | ASP | A   | 259    | 1.205  | 19.202 | 6.016  | 1.00  | 20.07 |
| ATOM | 1931 | OD2     | ASP | A   | 259    | 0.217  | 18.996 | 7.920  | 1.00  | 33.57 |
| ATOM | 1932 | C       | ASP | A   | 259    | 0.173  | 22.425 | 5.567  | 1.00  | 15.64 |
| ATOM | 1933 | O       | ASP | A   | 259    | -0.024 | 21.963 | 4.439  | 1.00  | 17.43 |
| ATOM | 1934 | N       | ARG | A   | 260    | -0.682 | 23.260 | 6.148  | 1.00  | 16.51 |
| ATOM | 1935 | CA      | ARG | A   | 260    | -1.947 | 23.632 | 5.504  | 1.00  | 16.62 |
| ATOM | 1936 | CB      | ARG | A   | 260    | -2.836 | 24.464 | 6.425  | 1.00  | 18.22 |
| ATOM | 1937 | CG      | ARG | A   | 260    | -3.435 | 23.668 | 7.571  | 1.00  | 25.51 |
| ATOM | 1938 | CD      | ARG | A   | 260    | -4.950 | 23.818 | 7.664  | 1.00  | 40.63 |
| ATOM | 1939 | NE      | ARG | A   | 260    | -5.428 | 25.199 | 7.581  | 1.00  | 49.41 |
| ATOM | 1940 | CZ      | ARG | A   | 260    | -5.919 | 25.797 | 6.491  | 1.00  | 52.56 |
| ATOM | 1941 | NH1     | ARG | A   | 260    | -6.025 | 25.176 | 5.311  | 1.00  | 50.50 |
| ATOM | 1942 | NH2     | ARG | A   | 260    | -6.310 | 27.059 | 6.592  | 1.00  | 53.49 |
| ATOM | 1943 | C       | ARG | A   | 260    | -1.685 | 24.431 | 4.233  | 1.00  | 16.45 |
| ATOM | 1944 | O       | ARG | A   | 260    | -2.247 | 24.131 | 3.165  | 1.00  | 18.96 |
| ATOM | 1945 | N       | ILE | A   | 261    | -0.767 | 25.394 | 4.310  | 1.00  | 15.77 |
| ATOM | 1946 | CA      | ILE | A   | 261    | -0.542 | 26.228 | 3.138  | 1.00  | 18.24 |
| ATOM | 1947 | CB      | ILE | A   | 261    | 0.206  | 27.521 | 3.521  | 1.00  | 21.96 |
| ATOM | 1948 | CG1AILE | A   | 261 | 1.651  | 27.329 | 3.908  | 0.50   | 17.99 |       |
| ATOM | 1949 | CG1BILE | A   | 261 | -0.685 | 28.609 | 4.112  | 0.50   | 19.62 |       |
| ATOM | 1950 | CD1AILE | A   | 261 | 2.215  | 28.633 | 4.442  | 0.50   | 20.12 |       |
| ATOM | 1951 | CD1BILE | A   | 261 | 0.000  | 29.266 | 5.315  | 0.50   | 24.86 |       |
| ATOM | 1952 | CG2AILE | A   | 261 | -0.604 | 28.289 | 4.549  | 0.50   | 18.49 |       |
| ATOM | 1953 | CG2BILE | A   | 261 | 1.211  | 27.966 | 2.472  | 0.50   | 19.26 |       |
| ATOM | 1954 | C       | ILE | A   | 261    | 0.067  | 25.456 | 1.973  | 1.00  | 19.50 |
| ATOM | 1955 | O       | ILE | A   | 261    | -0.278 | 25.684 | 0.799  | 1.00  | 17.34 |
| ATOM | 1956 | N       | LEU | A   | 262    | 1.002  | 24.564 | 2.291  | 1.00  | 18.57 |
| ATOM | 1957 | CA      | LEU | A   | 262    | 1.572  | 23.704 | 1.256  | 1.00  | 19.04 |
| ATOM | 1958 | CB      | LEU | A   | 262    | 2.736  | 22.874 | 1.776  | 1.00  | 17.43 |
| ATOM | 1959 | CG      | LEU | A   | 262    | 4.004  | 23.676 | 2.064  | 1.00  | 16.24 |
| ATOM | 1960 | CD1     | LEU | A   | 262    | 5.114  | 22.827 | 2.635  | 1.00  | 18.88 |
| ATOM | 1961 | CD2     | LEU | A   | 262    | 4.509  | 24.501 | 0.861  | 1.00  | 21.60 |
| ATOM | 1962 | C       | LEU | A   | 262    | 0.533  | 22.831 | 0.568  | 1.00  | 18.56 |
| ATOM | 1963 | O       | LEU | A   | 262    | 0.613  | 22.605 | -0.649 | 1.00  | 19.59 |
| ATOM | 1964 | N       | GLN | A   | 263    | -0.423 | 22.344 | 1.350  | 1.00  | 16.77 |
| ATOM | 1965 | CA      | GLN | A   | 263    | -1.517 | 21.572 | 0.772  | 1.00  | 18.98 |
| ATOM | 1966 | CB      | GLN | A   | 263    | -2.359 | 20.878 | 1.850  | 1.00  | 21.56 |
| ATOM | 1967 | CG      | GLN | A   | 263    | -1.581 | 19.736 | 2.499  | 1.00  | 24.14 |
| ATOM | 1968 | CD      | GLN | A   | 263    | -2.322 | 19.083 | 3.652  | 1.00  | 30.60 |
| ATOM | 1969 | OE1     | GLN | A   | 263    | -3.120 | 18.178 | 3.445  | 1.00  | 37.41 |
| ATOM | 1970 | NE2     | GLN | A   | 263    | -2.058 | 19.540 | 4.868  | 1.00  | 34.60 |
| ATOM | 1971 | C       | GLN | A   | 263    | -2.383 | 22.438 | -0.124 | 1.00  | 18.41 |
| ATOM | 1972 | O       | GLN | A   | 263    | -2.861 | 21.939 | -1.165 | 1.00  | 19.16 |
| ATOM | 1973 | N       | GLN | A   | 264    | -2.585 | 23.692 | 0.286  | 1.00  | 17.80 |
| ATOM | 1974 | CA      | GLN | A   | 264    | -3.284 | 24.667 | -0.547 | 1.00  | 19.17 |
| ATOM | 1975 | CB      | GLN | A   | 264    | -3.375 | 26.035 | 0.130  | 1.00  | 21.52 |

**FIGURE 290**

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|      |      |     |      |   |     |        |        |         |      |       |
|------|------|-----|------|---|-----|--------|--------|---------|------|-------|
| ATOM | 1976 | CG  | GLN  | A | 264 | -4.488 | 26.101 | 1.152   | 1.00 | 22.71 |
| ATOM | 1977 | CD  | GLN  | A | 264 | -4.485 | 27.392 | 1.924   | 1.00 | 27.25 |
| ATOM | 1978 | OE1 | GLN  | A | 264 | -3.974 | 28.404 | 1.452   | 1.00 | 28.01 |
| ATOM | 1979 | NE2 | GLN  | A | 264 | -5.062 | 27.364 | 3.126   | 1.00 | 32.99 |
| ATOM | 1980 | C   | GLN  | A | 264 | -2.569 | 24.866 | -1.856  | 1.00 | 17.97 |
| ATOM | 1981 | O   | GLN  | A | 264 | -3.195 | 24.854 | -2.914  | 1.00 | 18.97 |
| ATOM | 1982 | N   | LEU  | A | 265 | -1.243 | 25.044 | -1.807  | 1.00 | 16.73 |
| ATOM | 1983 | CA  | LEU  | A | 265 | -0.524 | 25.223 | -3.059  | 1.00 | 15.75 |
| ATOM | 1984 | CB  | LEU  | A | 265 | 0.944  | 25.599 | -2.792  | 1.00 | 16.04 |
| ATOM | 1985 | CG  | LEU  | A | 265 | 1.177  | 26.933 | -2.072  | 1.00 | 16.47 |
| ATOM | 1986 | CD1 | LEU  | A | 265 | 2.699  | 27.094 | -1.977  | 1.00 | 23.16 |
| ATOM | 1987 | CD2 | LEU  | A | 265 | 0.556  | 28.085 | -2.851  | 1.00 | 23.92 |
| ATOM | 1988 | C   | LEU  | A | 265 | -0.567 | 24.006 | -3.963  | 1.00 | 17.46 |
| ATOM | 1989 | O   | LEU  | A | 265 | -0.348 | 24.116 | -5.177  | 1.00 | 19.71 |
| ATOM | 1990 | N   | ASP  | A | 266 | -0.787 | 22.828 | -3.397  | 1.00 | 15.69 |
| ATOM | 1991 | CA  | ASP  | A | 266 | -0.767 | 21.626 | -4.210  | 1.00 | 16.88 |
| ATOM | 1992 | CB  | ASP  | A | 266 | -0.328 | 20.423 | -3.368  | 1.00 | 17.44 |
| ATOM | 1993 | CG  | ASP  | A | 266 | 1.156  | 20.375 | -3.149  | 1.00 | 21.62 |
| ATOM | 1994 | OD1 | ASP  | A | 266 | 1.862  | 21.159 | -3.791  | 1.00 | 21.03 |
| ATOM | 1995 | OD2 | ASP  | A | 266 | 1.680  | 19.586 | -2.335  | 1.00 | 25.07 |
| ATOM | 1996 | C   | ASP  | A | 266 | -2.163 | 21.343 | -4.768  | 1.00 | 16.49 |
| ATOM | 1997 | O   | ASP  | A | 266 | -2.320 | 20.469 | -5.624  | 1.00 | 18.65 |
| ATOM | 1998 | N   | SER  | A | 267 | -3.151 | 22.112 | -4.318  | 1.00 | 17.93 |
| ATOM | 1999 | CA  | SER  | A | 267 | -4.562 | 21.826 | -4.646  | 1.00 | 18.68 |
| ATOM | 2000 | CB  | SER  | A | 267 | -5.334 | 21.390 | -3.392  | 1.00 | 20.21 |
| ATOM | 2001 | OG  | ASER | A | 267 | -4.827 | 20.179 | -2.869  | 0.50 | 22.09 |
| ATOM | 2002 | OG  | BSER | A | 267 | -5.151 | 22.290 | -2.327  | 0.50 | 19.41 |
| ATOM | 2003 | C   | SER  | A | 267 | -5.375 | 22.910 | -5.354  | 1.00 | 19.44 |
| ATOM | 2004 | O   | SER  | A | 267 | -6.260 | 22.591 | -6.147  | 1.00 | 19.32 |
| ATOM | 2005 | N   | LYS  | A | 268 | -5.083 | 24.164 | -5.022  | 1.00 | 18.83 |
| ATOM | 2006 | CA  | LYS  | A | 268 | -5.848 | 25.354 | -5.377  | 1.00 | 20.16 |
| ATOM | 2007 | CB  | LYS  | A | 268 | -6.430 | 25.992 | -4.099  | 1.00 | 20.65 |
| ATOM | 2008 | CG  | LYS  | A | 268 | -7.498 | 25.094 | -3.470  | 1.00 | 26.76 |
| ATOM | 2009 | CD  | LYS  | A | 268 | -8.104 | 25.692 | -2.209  | 1.00 | 35.23 |
| ATOM | 2010 | CE  | LYS  | A | 268 | -9.065 | 26.845 | -2.493  | 1.00 | 39.80 |
| ATOM | 2011 | NZ  | LYS  | A | 268 | -9.302 | 27.654 | -1.258  | 1.00 | 42.30 |
| ATOM | 2012 | C   | LYS  | A | 268 | -4.995 | 26.373 | -6.115  | 1.00 | 20.26 |
| ATOM | 2013 | O   | LYS  | A | 268 | -3.762 | 26.340 | -6.077  | 1.00 | 20.14 |
| ATOM | 2014 | N   | ASP  | A | 269 | -5.653 | 27.329 | -6.766  | 1.00 | 20.67 |
| ATOM | 2015 | CA  | ASP  | A | 269 | -4.923 | 28.431 | -7.379  | 1.00 | 22.23 |
| ATOM | 2016 | CB  | ASP  | A | 269 | -5.354 | 28.695 | -8.824  | 1.00 | 21.86 |
| ATOM | 2017 | CG  | ASP  | A | 269 | -6.802 | 29.136 | -8.948  | 1.00 | 24.01 |
| ATOM | 2018 | OD1 | ASP  | A | 269 | -7.478 | 29.270 | -7.910  | 1.00 | 23.82 |
| ATOM | 2019 | OD2 | ASP  | A | 269 | -7.315 | 29.358 | -10.081 | 1.00 | 25.17 |
| ATOM | 2020 | C   | ASP  | A | 269 | -4.936 | 29.704 | -6.561  | 1.00 | 21.37 |
| ATOM | 2021 | O   | ASP  | A | 269 | -4.671 | 30.783 | -7.086  | 1.00 | 20.35 |
| ATOM | 2022 | N   | SER  | A | 270 | -5.235 | 29.557 | -5.272  | 1.00 | 22.33 |
| ATOM | 2023 | CA  | SER  | A | 270 | -5.009 | 30.638 | -4.323  | 1.00 | 20.47 |
| ATOM | 2024 | CB  | SER  | A | 270 | -6.278 | 31.451 | -4.075  | 1.00 | 24.06 |
| ATOM | 2025 | OG  | SER  | A | 270 | -7.314 | 30.640 | -3.578  | 1.00 | 26.40 |
| ATOM | 2026 | C   | SER  | A | 270 | -4.518 | 30.042 | -3.018  | 1.00 | 21.38 |
| ATOM | 2027 | O   | SER  | A | 270 | -4.735 | 28.852 | -2.739  | 1.00 | 22.73 |

**FIGURE 291**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2028 | N   | VAL | A | 271 | -3.885 | 30.903 | -2.225 | 1.00 | 22.36 |
| ATOM | 2029 | CA  | VAL | A | 271 | -3.263 | 30.508 | -0.963 | 1.00 | 21.09 |
| ATOM | 2030 | CB  | VAL | A | 271 | -1.709 | 30.463 | -1.115 | 1.00 | 19.31 |
| ATOM | 2031 | CG1 | VAL | A | 271 | -1.167 | 31.865 | -1.450 | 1.00 | 21.60 |
| ATOM | 2032 | CG2 | VAL | A | 271 | -1.082 | 29.972 | 0.200  | 1.00 | 21.85 |
| ATOM | 2033 | C   | VAL | A | 271 | -3.688 | 31.549 | 0.072  | 1.00 | 20.22 |
| ATOM | 2034 | O   | VAL | A | 271 | -3.787 | 32.736 | -0.240 | 1.00 | 22.08 |
| ATOM | 2035 | N   | ASP | A | 272 | -3.917 | 31.112 | 1.310  | 1.00 | 20.16 |
| ATOM | 2036 | CA  | ASP | A | 272 | -4.471 | 32.003 | 2.324  | 1.00 | 19.60 |
| ATOM | 2037 | CB  | ASP | A | 272 | -5.965 | 31.714 | 2.437  | 1.00 | 19.30 |
| ATOM | 2038 | CG  | ASP | A | 272 | -6.676 | 32.598 | 3.431  | 1.00 | 19.17 |
| ATOM | 2039 | OD1 | ASP | A | 272 | -6.077 | 33.593 | 3.891  | 1.00 | 21.60 |
| ATOM | 2040 | OD2 | ASP | A | 272 | -7.859 | 32.350 | 3.783  | 1.00 | 24.88 |
| ATOM | 2041 | C   | ASP | A | 272 | -3.744 | 31.805 | 3.655  | 1.00 | 20.36 |
| ATOM | 2042 | O   | ASP | A | 272 | -4.243 | 31.163 | 4.591  | 1.00 | 20.38 |
| ATOM | 2043 | N   | ILE | A | 273 | -2.541 | 32.365 | 3.720  | 1.00 | 19.70 |
| ATOM | 2044 | CA  | ILE | A | 273 | -1.760 | 32.311 | 4.942  | 1.00 | 19.19 |
| ATOM | 2045 | CB  | ILE | A | 273 | -0.381 | 32.962 | 4.720  | 1.00 | 18.60 |
| ATOM | 2046 | CG1 | ILE | A | 273 | 0.333  | 32.288 | 3.548  | 1.00 | 21.27 |
| ATOM | 2047 | CD1 | ILE | A | 273 | 1.729  | 32.865 | 3.275  | 1.00 | 22.60 |
| ATOM | 2048 | CG2 | ILE | A | 273 | 0.464  | 32.875 | 5.999  | 1.00 | 20.66 |
| ATOM | 2049 | C   | ILE | A | 273 | -2.477 | 32.966 | 6.107  | 1.00 | 20.28 |
| ATOM | 2050 | O   | ILE | A | 273 | -2.472 | 32.424 | 7.218  | 1.00 | 18.55 |
| ATOM | 2051 | N   | TYR | A | 274 | -3.100 | 34.117 | 5.869  | 1.00 | 18.83 |
| ATOM | 2052 | CA  | TYR | A | 274 | -3.766 | 34.840 | 6.953  | 1.00 | 21.01 |
| ATOM | 2053 | CB  | TYR | A | 274 | -4.367 | 36.112 | 6.356  | 1.00 | 19.87 |
| ATOM | 2054 | CG  | TYR | A | 274 | -5.067 | 36.972 | 7.358  | 1.00 | 18.97 |
| ATOM | 2055 | CD1 | TYR | A | 274 | -4.394 | 38.025 | 7.954  | 1.00 | 21.35 |
| ATOM | 2056 | CE1 | TYR | A | 274 | -5.029 | 38.859 | 8.864  | 1.00 | 25.25 |
| ATOM | 2057 | CZ  | TYR | A | 274 | -6.352 | 38.625 | 9.157  | 1.00 | 28.87 |
| ATOM | 2058 | OH  | TYR | A | 274 | -6.978 | 39.454 | 10.070 | 1.00 | 34.66 |
| ATOM | 2059 | CE2 | TYR | A | 274 | -7.051 | 37.579 | 8.579  | 1.00 | 26.00 |
| ATOM | 2060 | CD2 | TYR | A | 274 | -6.413 | 36.757 | 7.669  | 1.00 | 22.43 |
| ATOM | 2061 | C   | TYR | A | 274 | -4.875 | 33.977 | 7.550  | 1.00 | 21.55 |
| ATOM | 2062 | O   | TYR | A | 274 | -4.991 | 33.834 | 8.776  | 1.00 | 22.52 |
| ATOM | 2063 | N   | GLY | A | 275 | -5.625 | 33.326 | 6.671  | 1.00 | 19.33 |
| ATOM | 2064 | CA  | GLY | A | 275 | -6.741 | 32.496 | 7.090  | 1.00 | 19.21 |
| ATOM | 2065 | C   | GLY | A | 275 | -6.245 | 31.272 | 7.837  | 1.00 | 20.79 |
| ATOM | 2066 | O   | GLY | A | 275 | -6.889 | 30.859 | 8.796  | 1.00 | 22.44 |
| ATOM | 2067 | N   | ALA | A | 276 | -5.125 | 30.692 | 7.398  | 1.00 | 18.85 |
| ATOM | 2068 | CA  | ALA | A | 276 | -4.558 | 29.525 | 8.094  | 1.00 | 20.03 |
| ATOM | 2069 | CB  | ALA | A | 276 | -3.324 | 29.022 | 7.356  | 1.00 | 20.07 |
| ATOM | 2070 | C   | ALA | A | 276 | -4.195 | 29.870 | 9.542  | 1.00 | 19.85 |
| ATOM | 2071 | O   | ALA | A | 276 | -4.432 | 29.103 | 10.479 | 1.00 | 20.22 |
| ATOM | 2072 | N   | VAL | A | 277 | -3.537 | 31.010 | 9.719  | 1.00 | 19.70 |
| ATOM | 2073 | CA  | VAL | A | 277 | -3.115 | 31.387 | 11.057 | 1.00 | 19.31 |
| ATOM | 2074 | CB  | VAL | A | 277 | -2.121 | 32.548 | 11.018 | 1.00 | 17.79 |
| ATOM | 2075 | CG1 | VAL | A | 277 | -1.820 | 32.967 | 12.458 | 1.00 | 18.22 |
| ATOM | 2076 | CG2 | VAL | A | 277 | -0.848 | 32.152 | 10.255 | 1.00 | 18.41 |
| ATOM | 2077 | C   | VAL | A | 277 | -4.346 | 31.757 | 11.868 | 1.00 | 19.90 |
| ATOM | 2078 | O   | VAL | A | 277 | -4.474 | 31.347 | 13.019 | 1.00 | 20.30 |
| ATOM | 2079 | N   | HIS | A | 278 | -5.241 | 32.548 | 11.292 | 1.00 | 19.02 |

**FIGURE 292**



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|      |      |     |     |   |     |         |        |        |      |       |
|------|------|-----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 2080 | CA  | HIS | A | 278 | -6.516  | 32.865 | 11.948 | 1.00 | 19.17 |
| ATOM | 2081 | CB  | HIS | A | 278 | -7.444  | 33.619 | 10.992 | 1.00 | 19.25 |
| ATOM | 2082 | CG  | HIS | A | 278 | -8.751  | 33.994 | 11.601 | 1.00 | 18.26 |
| ATOM | 2083 | ND1 | HIS | A | 278 | -9.794  | 33.105 | 11.749 | 1.00 | 23.05 |
| ATOM | 2084 | CE1 | HIS | A | 278 | -10.818 | 33.721 | 12.311 | 1.00 | 21.29 |
| ATOM | 2085 | NE2 | HIS | A | 278 | -10.478 | 34.980 | 12.522 | 1.00 | 22.86 |
| ATOM | 2086 | CD2 | HIS | A | 278 | -9.189  | 35.176 | 12.093 | 1.00 | 20.74 |
| ATOM | 2087 | C   | HIS | A | 278 | -7.203  | 31.605 | 12.495 | 1.00 | 17.84 |
| ATOM | 2088 | O   | HIS | A | 278 | -7.537  | 31.525 | 13.680 | 1.00 | 18.09 |
| ATOM | 2089 | N   | ASP | A | 279 | -7.350  | 30.601 | 11.635 | 1.00 | 18.49 |
| ATOM | 2090 | CA  | ASP | A | 279 | -8.101  | 29.403 | 11.989 | 1.00 | 19.79 |
| ATOM | 2091 | CB  | ASP | A | 279 | -8.327  | 28.536 | 10.749 | 1.00 | 21.91 |
| ATOM | 2092 | CG  | ASP | A | 279 | -9.382  | 29.137 | 9.805  | 1.00 | 27.33 |
| ATOM | 2093 | OD1 | ASP | A | 279 | -10.122 | 30.086 | 10.181 | 1.00 | 32.69 |
| ATOM | 2094 | OD2 | ASP | A | 279 | -9.571  | 28.698 | 8.663  | 1.00 | 32.10 |
| ATOM | 2095 | C   | ASP | A | 279 | -7.376  | 28.645 | 13.092 | 1.00 | 19.96 |
| ATOM | 2096 | O   | ASP | A | 279 | -8.023  | 28.185 | 14.024 | 1.00 | 21.76 |
| ATOM | 2097 | N   | LEU | A | 280 | -6.040  | 28.527 | 13.041 | 1.00 | 17.01 |
| ATOM | 2098 | CA  | LEU | A | 280 | -5.330  | 27.942 | 14.182 | 1.00 | 16.07 |
| ATOM | 2099 | CB  | LEU | A | 280 | -3.826  | 27.947 | 13.886 | 1.00 | 15.00 |
| ATOM | 2100 | CG  | LEU | A | 280 | -3.422  | 27.038 | 12.707 | 1.00 | 18.81 |
| ATOM | 2101 | CD1 | LEU | A | 280 | -1.913  | 27.070 | 12.480 | 1.00 | 18.81 |
| ATOM | 2102 | CD2 | LEU | A | 280 | -3.882  | 25.608 | 12.945 | 1.00 | 25.24 |
| ATOM | 2103 | C   | LEU | A | 280 | -5.569  | 28.675 | 15.513 | 1.00 | 16.26 |
| ATOM | 2104 | O   | LEU | A | 280 | -5.712  | 28.053 | 16.564 | 1.00 | 16.85 |
| ATOM | 2105 | N   | ARG | A | 281 | -5.589  | 30.004 | 15.476 | 1.00 | 15.08 |
| ATOM | 2106 | CA  | ARG | A | 281 | -5.688  | 30.743 | 16.716 | 1.00 | 17.44 |
| ATOM | 2107 | CB  | ARG | A | 281 | -5.378  | 32.206 | 16.447 | 1.00 | 17.50 |
| ATOM | 2108 | CG  | ARG | A | 281 | -3.897  | 32.412 | 16.278 | 1.00 | 17.29 |
| ATOM | 2109 | CD  | ARG | A | 281 | -3.452  | 33.863 | 16.134 | 1.00 | 16.44 |
| ATOM | 2110 | NE  | ARG | A | 281 | -1.994  | 33.944 | 15.966 | 1.00 | 16.47 |
| ATOM | 2111 | CZ  | ARG | A | 281 | -1.298  | 35.076 | 15.842 | 1.00 | 18.10 |
| ATOM | 2112 | NH1 | ARG | A | 281 | -1.939  | 36.226 | 15.915 | 1.00 | 21.62 |
| ATOM | 2113 | NH2 | ARG | A | 281 | 0.034   | 35.066 | 15.648 | 1.00 | 18.29 |
| ATOM | 2114 | C   | ARG | A | 281 | -7.060  | 30.626 | 17.353 | 1.00 | 17.49 |
| ATOM | 2115 | O   | ARG | A | 281 | -7.199  | 30.854 | 18.553 | 1.00 | 19.29 |
| ATOM | 2116 | N   | LEU | A | 282 | -8.062  | 30.261 | 16.560 | 1.00 | 18.15 |
| ATOM | 2117 | CA  | LEU | A | 282 | -9.358  | 29.983 | 17.142 | 1.00 | 17.68 |
| ATOM | 2118 | CB  | LEU | A | 282 | -10.396 | 29.682 | 16.062 | 1.00 | 16.99 |
| ATOM | 2119 | CG  | LEU | A | 282 | -10.801 | 30.873 | 15.182 | 1.00 | 19.43 |
| ATOM | 2120 | CD1 | LEU | A | 282 | -11.737 | 30.362 | 14.090 | 1.00 | 25.48 |
| ATOM | 2121 | CD2 | LEU | A | 282 | -11.501 | 31.952 | 16.018 | 1.00 | 24.65 |
| ATOM | 2122 | C   | LEU | A | 282 | -9.279  | 28.793 | 18.102 | 1.00 | 19.14 |
| ATOM | 2123 | O   | LEU | A | 282 | -10.141 | 28.668 | 18.977 | 1.00 | 19.96 |
| ATOM | 2124 | N   | HIS | A | 283 | -8.293  | 27.918 | 17.896 | 1.00 | 17.18 |
| ATOM | 2125 | CA  | HIS | A | 283 | -8.277  | 26.637 | 18.601 | 1.00 | 18.07 |
| ATOM | 2126 | CB  | HIS | A | 283 | -8.139  | 25.490 | 17.597 | 1.00 | 18.24 |
| ATOM | 2127 | CG  | HIS | A | 283 | -9.231  | 25.476 | 16.585 | 1.00 | 19.11 |
| ATOM | 2128 | ND1 | HIS | A | 283 | -10.466 | 24.910 | 16.822 | 1.00 | 23.60 |
| ATOM | 2129 | CE1 | HIS | A | 283 | -11.231 | 25.064 | 15.756 | 1.00 | 19.21 |
| ATOM | 2130 | NE2 | HIS | A | 283 | -10.545 | 25.722 | 14.844 | 1.00 | 24.32 |
| ATOM | 2131 | CD2 | HIS | A | 283 | -9.296  | 26.007 | 15.343 | 1.00 | 23.68 |

**FIGURE 293**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2132 | C   | HIS | A | 283 | -7.254 | 26.512 | 19.707 | 1.00 | 17.83 |
| ATOM | 2133 | O   | HIS | A | 283 | -7.428 | 25.694 | 20.622 | 1.00 | 18.19 |
| ATOM | 2134 | N   | ARG | A | 284 | -6.201 | 27.314 | 19.637 | 1.00 | 17.80 |
| ATOM | 2135 | CA  | ARG | A | 284 | -5.240 | 27.348 | 20.746 | 1.00 | 18.49 |
| ATOM | 2136 | CB  | ARG | A | 284 | -4.226 | 26.210 | 20.609 | 1.00 | 18.69 |
| ATOM | 2137 | CG  | ARG | A | 284 | -3.276 | 26.099 | 21.796 | 1.00 | 18.21 |
| ATOM | 2138 | CD  | ARG | A | 284 | -2.402 | 24.878 | 21.679 | 1.00 | 19.61 |
| ATOM | 2139 | NE  | ARG | A | 284 | -1.291 | 24.852 | 22.639 | 1.00 | 17.43 |
| ATOM | 2140 | CZ  | ARG | A | 284 | -1.355 | 24.269 | 23.836 | 1.00 | 15.60 |
| ATOM | 2141 | NH1 | ARG | A | 284 | -2.509 | 23.773 | 24.275 | 1.00 | 16.53 |
| ATOM | 2142 | NH2 | ARG | A | 284 | -0.290 | 24.237 | 24.619 | 1.00 | 17.46 |
| ATOM | 2143 | C   | ARG | A | 284 | -4.530 | 28.695 | 20.752 | 1.00 | 17.37 |
| ATOM | 2144 | O   | ARG | A | 284 | -4.367 | 29.323 | 19.707 | 1.00 | 16.68 |
| ATOM | 2145 | N   | VAL | A | 285 | -4.142 | 29.123 | 21.941 | 1.00 | 16.77 |
| ATOM | 2146 | CA  | VAL | A | 285 | -3.720 | 30.502 | 22.158 | 1.00 | 18.62 |
| ATOM | 2147 | CB  | VAL | A | 285 | -3.294 | 30.774 | 23.616 | 1.00 | 18.24 |
| ATOM | 2148 | CG1 | VAL | A | 285 | -2.160 | 29.860 | 24.061 | 1.00 | 18.15 |
| ATOM | 2149 | CG2 | VAL | A | 285 | -2.946 | 32.249 | 23.792 | 1.00 | 21.76 |
| ATOM | 2150 | C   | VAL | A | 285 | -2.599 | 30.925 | 21.225 | 1.00 | 19.42 |
| ATOM | 2151 | O   | VAL | A | 285 | -1.503 | 30.358 | 21.256 | 1.00 | 20.43 |
| ATOM | 2152 | N   | HIS | A | 286 | -2.914 | 31.919 | 20.395 | 1.00 | 21.27 |
| ATOM | 2153 | CA  | HIS | A | 286 | -1.916 | 32.671 | 19.615 | 1.00 | 22.02 |
| ATOM | 2154 | CB  | HIS | A | 286 | -1.237 | 33.690 | 20.547 | 1.00 | 20.50 |
| ATOM | 2155 | CG  | HIS | A | 286 | -0.509 | 34.803 | 19.848 | 1.00 | 23.00 |
| ATOM | 2156 | ND1 | HIS | A | 286 | 0.558  | 34.583 | 19.001 | 1.00 | 22.19 |
| ATOM | 2157 | CE1 | HIS | A | 286 | 0.997  | 35.742 | 18.539 | 1.00 | 28.42 |
| ATOM | 2158 | NE2 | HIS | A | 286 | 0.299  | 36.711 | 19.104 | 1.00 | 23.08 |
| ATOM | 2159 | CD2 | HIS | A | 286 | -0.660 | 36.149 | 19.920 | 1.00 | 25.08 |
| ATOM | 2160 | C   | HIS | A | 286 | -0.937 | 31.748 | 18.880 | 1.00 | 20.60 |
| ATOM | 2161 | O   | HIS | A | 286 | 0.249  | 32.021 | 18.774 | 1.00 | 22.19 |
| ATOM | 2162 | N   | MET | A | 287 | -1.425 | 30.634 | 18.328 | 1.00 | 19.66 |
| ATOM | 2163 | CA  | MET | A | 287 | -0.622 | 29.854 | 17.395 | 1.00 | 20.00 |
| ATOM | 2164 | CB  | MET | A | 287 | -1.505 | 28.919 | 16.577 | 1.00 | 21.36 |
| ATOM | 2165 | CG  | MET | A | 287 | -2.213 | 27.872 | 17.401 | 1.00 | 22.55 |
| ATOM | 2166 | SD  | MET | A | 287 | -1.075 | 26.566 | 17.823 | 1.00 | 40.15 |
| ATOM | 2167 | CE  | MET | A | 287 | -1.223 | 27.071 | 19.109 | 1.00 | 6.08  |
| ATOM | 2168 | C   | MET | A | 287 | 0.133  | 30.710 | 16.385 | 1.00 | 20.09 |
| ATOM | 2169 | O   | MET | A | 287 | -0.471 | 31.515 | 15.681 | 1.00 | 20.94 |
| ATOM | 2170 | N   | VAL | A | 288 | 1.422  | 30.424 | 16.237 | 1.00 | 19.63 |
| ATOM | 2171 | CA  | VAL | A | 288 | 2.388  | 31.249 | 15.511 | 1.00 | 18.83 |
| ATOM | 2172 | CB  | VAL | A | 288 | 1.962  | 31.725 | 14.093 | 1.00 | 17.58 |
| ATOM | 2173 | CG1 | VAL | A | 288 | 3.180  | 32.328 | 13.410 | 1.00 | 18.31 |
| ATOM | 2174 | CG2 | VAL | A | 288 | 1.542  | 30.563 | 13.204 | 1.00 | 17.78 |
| ATOM | 2175 | C   | VAL | A | 288 | 2.758  | 32.425 | 16.439 | 1.00 | 18.47 |
| ATOM | 2176 | O   | VAL | A | 288 | 1.937  | 33.283 | 16.710 | 1.00 | 20.51 |
| ATOM | 2177 | N   | GLN | A | 289 | 3.970  | 32.397 | 16.978 | 1.00 | 20.96 |
| ATOM | 2178 | CA  | GLN | A | 289 | 4.275  | 33.242 | 18.136 | 1.00 | 22.85 |
| ATOM | 2179 | CB  | GLN | A | 289 | 5.360  | 32.573 | 18.989 | 1.00 | 23.05 |
| ATOM | 2180 | CG  | GLN | A | 289 | 5.711  | 33.382 | 20.255 | 1.00 | 23.08 |
| ATOM | 2181 | CD  | GLN | A | 289 | 6.940  | 32.853 | 20.982 | 1.00 | 24.28 |
| ATOM | 2182 | OE1 | GLN | A | 289 | 7.913  | 32.445 | 20.361 | 1.00 | 27.56 |
| ATOM | 2183 | NE2 | GLN | A | 289 | 6.888  | 32.843 | 22.309 | 1.00 | 23.63 |

**FIGURE 294**

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2184 | C   | GLN | A | 289 | 4.723  | 34.660 | 17.707 | 1.00 | 24.40 |
| ATOM | 2185 | O   | GLN | A | 289 | 4.391  | 35.649 | 18.378 | 1.00 | 23.35 |
| ATOM | 2186 | N   | THR | A | 290 | 5.492  | 34.737 | 16.617 | 1.00 | 26.49 |
| ATOM | 2187 | CA  | THR | A | 290 | 6.172  | 35.968 | 16.207 | 1.00 | 25.39 |
| ATOM | 2188 | CB  | THR | A | 290 | 7.702  | 35.856 | 16.359 | 1.00 | 26.91 |
| ATOM | 2189 | OG1 | THR | A | 290 | 8.244  | 35.042 | 15.307 | 1.00 | 28.99 |
| ATOM | 2190 | CG2 | THR | A | 290 | 8.109  | 35.128 | 17.629 | 1.00 | 27.48 |
| ATOM | 2191 | C   | THR | A | 290 | 5.866  | 36.465 | 14.801 | 1.00 | 26.87 |
| ATOM | 2192 | O   | THR | A | 290 | 5.512  | 35.692 | 13.896 | 1.00 | 25.17 |
| ATOM | 2193 | N   | GLU | A | 291 | 6.023  | 37.770 | 14.595 | 1.00 | 25.95 |
| ATOM | 2194 | CA  | GLU | A | 291 | 5.904  | 38.299 | 13.242 | 1.00 | 26.94 |
| ATOM | 2195 | CB  | GLU | A | 291 | 6.101  | 39.818 | 13.221 | 1.00 | 28.49 |
| ATOM | 2196 | CG  | GLU | A | 291 | 5.769  | 40.445 | 11.874 | 1.00 | 26.87 |
| ATOM | 2197 | CD  | GLU | A | 291 | 6.009  | 41.941 | 11.858 | 1.00 | 36.69 |
| ATOM | 2198 | OE1 | GLU | A | 291 | 7.008  | 42.378 | 11.254 | 1.00 | 43.24 |
| ATOM | 2199 | OE2 | GLU | A | 291 | 5.212  | 42.677 | 12.471 | 1.00 | 40.46 |
| ATOM | 2200 | C   | GLU | A | 291 | 6.910  | 37.609 | 12.314 | 1.00 | 26.09 |
| ATOM | 2201 | O   | GLU | A | 291 | 6.577  | 37.275 | 11.174 | 1.00 | 25.81 |
| ATOM | 2202 | N   | CYS | A | 292 | 8.123  | 37.346 | 12.792 | 1.00 | 27.35 |
| ATOM | 2203 | CA  | CYS | A | 292 | 9.115  | 36.718 | 11.917 | 1.00 | 27.95 |
| ATOM | 2204 | CB  | CYS | A | 292 | 10.448 | 36.520 | 12.615 | 1.00 | 29.85 |
| ATOM | 2205 | SG  | CYS | A | 292 | 11.241 | 38.119 | 12.768 | 1.00 | 41.05 |
| ATOM | 2206 | C   | CYS | A | 292 | 8.623  | 35.388 | 11.374 | 1.00 | 24.32 |
| ATOM | 2207 | O   | CYS | A | 292 | 8.866  | 35.043 | 10.217 | 1.00 | 21.58 |
| ATOM | 2208 | N   | GLN | A | 293 | 7.928  | 34.654 | 12.234 | 1.00 | 23.27 |
| ATOM | 2209 | CA  | GLN | A | 293 | 7.384  | 33.358 | 11.845 | 1.00 | 22.22 |
| ATOM | 2210 | CB  | GLN | A | 293 | 6.829  | 32.657 | 13.092 | 1.00 | 23.15 |
| ATOM | 2211 | CG  | GLN | A | 293 | 7.935  | 32.014 | 13.943 | 1.00 | 22.95 |
| ATOM | 2212 | CD  | GLN | A | 293 | 7.497  | 31.584 | 15.342 | 1.00 | 24.04 |
| ATOM | 2213 | OE1 | GLN | A | 293 | 6.342  | 31.765 | 15.721 | 1.00 | 21.47 |
| ATOM | 2214 | NE2 | GLN | A | 293 | 8.409  | 30.964 | 16.098 | 1.00 | 21.01 |
| ATOM | 2215 | C   | GLN | A | 293 | 6.316  | 33.548 | 10.766 | 1.00 | 21.55 |
| ATOM | 2216 | O   | GLN | A | 293 | 6.228  | 32.792 | 9.791  | 1.00 | 20.32 |
| ATOM | 2217 | N   | TYR | A | 294 | 5.506  | 34.586 | 10.920 | 1.00 | 21.97 |
| ATOM | 2218 | CA  | TYR | A | 294 | 4.537  | 34.924 | 9.888  | 1.00 | 21.49 |
| ATOM | 2219 | CB  | TYR | A | 294 | 3.670  | 36.091 | 10.352 | 1.00 | 23.10 |
| ATOM | 2220 | CG  | TYR | A | 294 | 2.400  | 36.319 | 9.556  | 1.00 | 21.89 |
| ATOM | 2221 | CD1 | TYR | A | 294 | 1.379  | 35.379 | 9.531  | 1.00 | 19.98 |
| ATOM | 2222 | CE1 | TYR | A | 294 | 0.185  | 35.606 | 8.862  | 1.00 | 22.15 |
| ATOM | 2223 | CZ  | TYR | A | 294 | 0.045  | 36.772 | 8.138  | 1.00 | 24.71 |
| ATOM | 2224 | OH  | TYR | A | 294 | -1.116 | 36.991 | 7.445  | 1.00 | 25.08 |
| ATOM | 2225 | CE2 | TYR | A | 294 | 1.059  | 37.703 | 8.118  | 1.00 | 22.86 |
| ATOM | 2226 | CD2 | TYR | A | 294 | 2.222  | 37.489 | 8.827  | 1.00 | 23.52 |
| ATOM | 2227 | C   | TYR | A | 294 | 5.239  | 35.306 | 8.576  | 1.00 | 22.57 |
| ATOM | 2228 | O   | TYR | A | 294 | 4.786  | 34.933 | 7.491  | 1.00 | 20.32 |
| ATOM | 2229 | N   | VAL | A | 295 | 6.373  | 36.001 | 8.670  | 1.00 | 22.24 |
| ATOM | 2230 | CA  | VAL | A | 295 | 7.104  | 36.358 | 7.454  | 1.00 | 20.86 |
| ATOM | 2231 | CB  | VAL | A | 295 | 8.267  | 37.326 | 7.712  | 1.00 | 23.76 |
| ATOM | 2232 | CG1 | VAL | A | 295 | 9.018  | 37.568 | 6.381  | 1.00 | 23.08 |
| ATOM | 2233 | CG2 | VAL | A | 295 | 7.749  | 38.634 | 8.308  | 1.00 | 23.92 |
| ATOM | 2234 | C   | VAL | A | 295 | 7.640  | 35.093 | 6.790  | 1.00 | 19.44 |
| ATOM | 2235 | O   | VAL | A | 295 | 7.633  | 34.973 | 5.572  | 1.00 | 20.82 |

**FIGURE 295**

Evdokimov et al. 9045M2  
Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |        |      |       |
|------|------|-----|-----|---|-----|--------|--------|--------|------|-------|
| ATOM | 2236 | N   | TYR | A | 296 | 8.078  | 34.149 | 7.611  | 1.00 | 21.43 |
| ATOM | 2237 | CA  | TYR | A | 296 | 8.763  | 32.971 | 7.121  | 1.00 | 19.39 |
| ATOM | 2238 | CB  | TYR | A | 296 | 9.281  | 32.156 | 8.298  | 1.00 | 19.80 |
| ATOM | 2239 | CG  | TYR | A | 296 | 9.911  | 30.860 | 7.902  | 1.00 | 18.43 |
| ATOM | 2240 | CD1 | TYR | A | 296 | 11.208 | 30.833 | 7.381  | 1.00 | 18.72 |
| ATOM | 2241 | CE1 | TYR | A | 296 | 11.823 | 29.631 | 7.077  | 1.00 | 22.90 |
| ATOM | 2242 | CZ  | TYR | A | 296 | 11.154 | 28.450 | 7.332  | 1.00 | 22.92 |
| ATOM | 2243 | OH  | TYR | A | 296 | 11.728 | 27.247 | 7.033  | 1.00 | 23.22 |
| ATOM | 2244 | CE2 | TYR | A | 296 | 9.873  | 28.447 | 7.854  | 1.00 | 21.43 |
| ATOM | 2245 | CD2 | TYR | A | 296 | 9.275  | 29.644 | 8.162  | 1.00 | 21.11 |
| ATOM | 2246 | C   | TYR | A | 296 | 7.771  | 32.136 | 6.320  | 1.00 | 18.46 |
| ATOM | 2247 | O   | TYR | A | 296 | 8.157  | 31.542 | 5.319  | 1.00 | 19.77 |
| ATOM | 2248 | N   | LEU | A | 297 | 6.509  | 32.096 | 6.767  | 1.00 | 19.80 |
| ATOM | 2249 | CA  | LEU | A | 297 | 5.478  | 31.346 | 6.056  | 1.00 | 17.52 |
| ATOM | 2250 | CB  | LEU | A | 297 | 4.148  | 31.412 | 6.825  | 1.00 | 19.78 |
| ATOM | 2251 | CG  | LEU | A | 297 | 4.110  | 30.542 | 8.092  | 1.00 | 16.59 |
| ATOM | 2252 | CD1 | LEU | A | 297 | 2.768  | 30.733 | 8.798  | 1.00 | 20.00 |
| ATOM | 2253 | CD2 | LEU | A | 297 | 4.304  | 29.063 | 7.757  | 1.00 | 18.37 |
| ATOM | 2254 | C   | LEU | A | 297 | 5.311  | 31.947 | 4.657  | 1.00 | 18.94 |
| ATOM | 2255 | O   | LEU | A | 297 | 5.174  | 31.247 | 3.654  | 1.00 | 19.58 |
| ATOM | 2256 | N   | HIS | A | 298 | 5.350  | 33.270 | 4.588  | 1.00 | 19.76 |
| ATOM | 2257 | CA  | HIS | A | 298 | 5.257  | 33.950 | 3.290  | 1.00 | 19.33 |
| ATOM | 2258 | CB  | HIS | A | 298 | 5.120  | 35.462 | 3.508  | 1.00 | 20.79 |
| ATOM | 2259 | CG  | HIS | A | 298 | 3.742  | 35.888 | 3.889  | 1.00 | 19.70 |
| ATOM | 2260 | ND1 | HIS | A | 298 | 3.242  | 35.727 | 5.165  | 1.00 | 20.71 |
| ATOM | 2261 | CE1 | HIS | A | 298 | 1.991  | 36.153 | 5.195  | 1.00 | 20.63 |
| ATOM | 2262 | NE2 | HIS | A | 298 | 1.672  | 36.608 | 3.998  | 1.00 | 23.44 |
| ATOM | 2263 | CD2 | HIS | A | 298 | 2.753  | 36.453 | 3.162  | 1.00 | 20.17 |
| ATOM | 2264 | C   | HIS | A | 298 | 6.475  | 33.665 | 2.410  | 1.00 | 18.63 |
| ATOM | 2265 | O   | HIS | A | 298 | 6.333  | 33.486 | 1.200  | 1.00 | 20.17 |
| ATOM | 2266 | N   | GLN | A | 299 | 7.667  | 33.627 | 2.990  | 1.00 | 21.31 |
| ATOM | 2267 | CA  | GLN | A | 299 | 8.868  | 33.309 | 2.226  | 1.00 | 20.83 |
| ATOM | 2268 | CB  | GLN | A | 299 | 10.128 | 33.492 | 3.082  | 1.00 | 22.50 |
| ATOM | 2269 | CG  | GLN | A | 299 | 10.312 | 34.954 | 3.499  | 1.00 | 25.27 |
| ATOM | 2270 | CD  | GLN | A | 299 | 11.423 | 35.135 | 4.525  | 1.00 | 28.26 |
| ATOM | 2271 | OE1 | GLN | A | 299 | 11.557 | 34.329 | 5.445  | 1.00 | 29.83 |
| ATOM | 2272 | NE2 | GLN | A | 299 | 12.188 | 36.219 | 4.403  | 1.00 | 26.71 |
| ATOM | 2273 | C   | GLN | A | 299 | 8.769  | 31.887 | 1.693  | 1.00 | 21.19 |
| ATOM | 2274 | O   | GLN | A | 299 | 9.147  | 31.646 | 0.552  | 1.00 | 20.84 |
| ATOM | 2275 | N   | CYS | A | 300 | 8.231  | 30.964 | 2.490  | 1.00 | 19.77 |
| ATOM | 2276 | CA  | CYS | A | 300 | 8.097  | 29.590 | 2.021  | 1.00 | 21.20 |
| ATOM | 2277 | CB  | CYS | A | 300 | 7.546  | 28.649 | 3.111  | 1.00 | 21.59 |
| ATOM | 2278 | SG  | CYS | A | 300 | 8.659  | 28.313 | 4.496  | 1.00 | 21.31 |
| ATOM | 2279 | C   | CYS | A | 300 | 7.227  | 29.549 | 0.778  | 1.00 | 18.38 |
| ATOM | 2280 | O   | CYS | A | 300 | 7.572  | 28.916 | -0.213 | 1.00 | 19.58 |
| ATOM | 2281 | N   | VAL | A | 301 | 6.076  | 30.207 | 0.833  | 1.00 | 20.07 |
| ATOM | 2282 | CA  | VAL | A | 301 | 5.143  | 30.161 | -0.279 | 1.00 | 19.34 |
| ATOM | 2283 | CB  | VAL | A | 301 | 3.831  | 30.847 | 0.087  | 1.00 | 19.69 |
| ATOM | 2284 | CG1 | VAL | A | 301 | 2.980  | 31.013 | -1.147 | 1.00 | 19.02 |
| ATOM | 2285 | CG2 | VAL | A | 301 | 3.082  | 30.041 | 1.150  | 1.00 | 23.02 |
| ATOM | 2286 | C   | VAL | A | 301 | 5.730  | 30.824 | -1.522 | 1.00 | 18.98 |
| ATOM | 2287 | O   | VAL | A | 301 | 5.634  | 30.294 | -2.652 | 1.00 | 18.99 |

**FIGURE 296**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |         |      |       |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2288 | N   | ARG | A | 302 | 6.361  | 31.968 | -1.289  | 1.00 | 20.60 |
| ATOM | 2289 | CA  | ARG | A | 302 | 7.085  | 32.662 | -2.365  | 1.00 | 22.52 |
| ATOM | 2290 | CB  | ARG | A | 302 | 7.807  | 33.876 | -1.811  | 1.00 | 23.52 |
| ATOM | 2291 | CG  | ARG | A | 302 | 8.616  | 34.611 | -2.872  | 1.00 | 24.32 |
| ATOM | 2292 | CD  | ARG | A | 302 | 9.710  | 35.455 | -2.228  | 1.00 | 26.13 |
| ATOM | 2293 | NE  | ARG | A | 302 | 10.667 | 34.616 | -1.520  | 1.00 | 31.05 |
| ATOM | 2294 | CZ  | ARG | A | 302 | 11.476 | 35.050 | -0.558  | 1.00 | 36.30 |
| ATOM | 2295 | NH1 | ARG | A | 302 | 11.460 | 36.326 | -0.192  | 1.00 | 37.18 |
| ATOM | 2296 | NH2 | ARG | A | 302 | 12.305 | 34.207 | 0.041   | 1.00 | 34.04 |
| ATOM | 2297 | C   | ARG | A | 302 | 8.087  | 31.777 | -3.095  | 1.00 | 23.40 |
| ATOM | 2298 | O   | ARG | A | 302 | 8.103  | 31.755 | -4.329  | 1.00 | 23.55 |
| ATOM | 2299 | N   | ASP | A | 303 | 8.903  | 31.055 | -2.328  | 1.00 | 22.39 |
| ATOM | 2300 | CA  | ASP | A | 303 | 9.904  | 30.144 | -2.863  | 1.00 | 22.73 |
| ATOM | 2301 | CB  | ASP | A | 303 | 10.892 | 29.686 | -1.773  | 1.00 | 21.26 |
| ATOM | 2302 | CG  | ASP | A | 303 | 11.711 | 30.827 | -1.192  | 1.00 | 28.53 |
| ATOM | 2303 | OD1 | ASP | A | 303 | 11.710 | 31.931 | -1.789  | 1.00 | 27.62 |
| ATOM | 2304 | OD2 | ASP | A | 303 | 12.386 | 30.699 | -0.137  | 1.00 | 26.66 |
| ATOM | 2305 | C   | ASP | A | 303 | 9.338  | 28.944 | -3.632  | 1.00 | 20.36 |
| ATOM | 2306 | O   | ASP | A | 303 | 9.838  | 28.603 | -4.712  | 1.00 | 21.25 |
| ATOM | 2307 | N   | VAL | A | 304 | 8.284  | 28.318 | -3.106  | 1.00 | 20.24 |
| ATOM | 2308 | CA  | VAL | A | 304 | 7.656  | 27.200 | -3.805  | 1.00 | 19.03 |
| ATOM | 2309 | CB  | VAL | A | 304 | 6.506  | 26.614 | -2.948  | 1.00 | 21.99 |
| ATOM | 2310 | CG1 | VAL | A | 304 | 5.687  | 25.599 | -3.724  | 1.00 | 21.81 |
| ATOM | 2311 | CG2 | VAL | A | 304 | 7.116  | 25.982 | -1.713  | 1.00 | 22.11 |
| ATOM | 2312 | C   | VAL | A | 304 | 7.141  | 27.710 | -5.149  | 1.00 | 19.92 |
| ATOM | 2313 | O   | VAL | A | 304 | 7.322  | 27.066 | -6.197  | 1.00 | 21.24 |
| ATOM | 2314 | N   | LEU | A | 305 | 6.459  | 28.851 | -5.112  | 1.00 | 18.22 |
| ATOM | 2315 | CA  | LEU | A | 305 | 5.836  | 29.364 | -6.332  | 1.00 | 20.56 |
| ATOM | 2316 | CB  | LEU | A | 305 | 4.844  | 30.480 | -6.012  | 1.00 | 17.57 |
| ATOM | 2317 | CG  | LEU | A | 305 | 3.557  | 30.008 | -5.320  | 1.00 | 19.17 |
| ATOM | 2318 | CD1 | LEU | A | 305 | 2.712  | 31.253 | -4.985  | 1.00 | 19.55 |
| ATOM | 2319 | CD2 | LEU | A | 305 | 2.691  | 28.974 | -6.082  | 1.00 | 20.38 |
| ATOM | 2320 | C   | LEU | A | 305 | 6.824  | 29.794 | -7.407  | 1.00 | 21.36 |
| ATOM | 2321 | O   | LEU | A | 305 | 6.574  | 29.576 | -8.606  | 1.00 | 23.65 |
| ATOM | 2322 | N   | ARG | A | 306 | 7.947  | 30.358 | -6.969  | 1.00 | 23.97 |
| ATOM | 2323 | CA  | ARG | A | 306 | 9.014  | 30.735 | -7.913  | 1.00 | 23.57 |
| ATOM | 2324 | CB  | ARG | A | 306 | 10.171 | 31.436 | -7.207  | 1.00 | 23.85 |
| ATOM | 2325 | CG  | ARG | A | 306 | 9.941  | 32.875 | -6.733  | 1.00 | 26.18 |
| ATOM | 2326 | CD  | ARG | A | 306 | 11.158 | 33.484 | -6.039  | 1.00 | 35.81 |
| ATOM | 2327 | NE  | ARG | A | 306 | 11.010 | 34.920 | -5.779  | 1.00 | 36.91 |
| ATOM | 2328 | CZ  | ARG | A | 306 | 11.865 | 35.646 | -5.060  | 1.00 | 37.77 |
| ATOM | 2329 | NH1 | ARG | A | 306 | 12.925 | 35.079 | -4.500  | 1.00 | 36.45 |
| ATOM | 2330 | NH2 | ARG | A | 306 | 11.658 | 36.947 | -4.882  | 1.00 | 37.40 |
| ATOM | 2331 | C   | ARG | A | 306 | 9.547  | 29.478 | -8.604  | 1.00 | 25.69 |
| ATOM | 2332 | O   | ARG | A | 306 | 9.712  | 29.439 | -9.834  | 1.00 | 23.35 |
| ATOM | 2333 | N   | ALA | A | 307 | 9.792  | 28.436 | -7.811  | 1.00 | 23.29 |
| ATOM | 2334 | CA  | ALA | A | 307 | 10.314 | 27.185 | -8.349  | 1.00 | 24.26 |
| ATOM | 2335 | CB  | ALA | A | 307 | 10.556 | 26.230 | -7.205  | 1.00 | 24.03 |
| ATOM | 2336 | C   | ALA | A | 307 | 9.354  | 26.565 | -9.344  | 1.00 | 22.10 |
| ATOM | 2337 | O   | ALA | A | 307 | 9.740  | 26.077 | -10.410 | 1.00 | 22.72 |
| ATOM | 2338 | N   | ARG | A | 308 | 8.068  | 26.598 | -9.008  | 1.00 | 20.80 |
| ATOM | 2339 | CA  | ARG | A | 308 | 7.092  | 25.915 | -9.835  | 1.00 | 20.00 |

**FIGURE 297**

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Three Dimensional Coordinates of HPTPbeta

|      |      |     |     |   |     |        |        |         |      |       |
|------|------|-----|-----|---|-----|--------|--------|---------|------|-------|
| ATOM | 2340 | CB  | ARG | A | 308 | 5.774  | 25.772 | -9.075  | 1.00 | 21.72 |
| ATOM | 2341 | CG  | ARG | A | 308 | 5.870  | 24.610 | -8.109  | 1.00 | 22.26 |
| ATOM | 2342 | CD  | ARG | A | 308 | 4.618  | 24.345 | -7.299  | 1.00 | 19.97 |
| ATOM | 2343 | NE  | ARG | A | 308 | 4.902  | 23.149 | -6.503  | 1.00 | 24.07 |
| ATOM | 2344 | CZ  | ARG | A | 308 | 4.025  | 22.542 | -5.718  | 1.00 | 27.19 |
| ATOM | 2345 | NH1 | ARG | A | 308 | 2.791  | 23.003 | -5.673  | 1.00 | 23.93 |
| ATOM | 2346 | NH2 | ARG | A | 308 | 4.377  | 21.464 | -5.012  | 1.00 | 28.78 |
| ATOM | 2347 | C   | ARG | A | 308 | 6.876  | 26.662 | -11.139 | 1.00 | 22.15 |
| ATOM | 2348 | O   | ARG | A | 308 | 6.699  | 26.030 | -12.176 | 1.00 | 21.30 |
| ATOM | 2349 | N   | LYS | A | 309 | 6.953  | 27.992 | -11.082 | 1.00 | 21.16 |
| ATOM | 2350 | CA  | LYS | A | 309 | 6.685  | 28.832 | -12.253 | 1.00 | 22.32 |
| ATOM | 2351 | CB  | LYS | A | 309 | 6.801  | 30.333 | -11.901 | 1.00 | 24.02 |
| ATOM | 2352 | CG  | LYS | A | 309 | 6.508  | 31.340 | -13.040 | 1.00 | 29.43 |
| ATOM | 2353 | CD  | LYS | A | 309 | 6.215  | 32.737 | -12.484 | 1.00 | 37.46 |
| ATOM | 2354 | CE  | LYS | A | 309 | 5.642  | 33.687 | -13.538 | 1.00 | 44.02 |
| ATOM | 2355 | NZ  | LYS | A | 309 | 6.468  | 34.926 | -13.712 | 1.00 | 43.80 |
| ATOM | 2356 | C   | LYS | A | 309 | 7.656  | 28.466 | -13.367 | 1.00 | 22.56 |
| ATOM | 2357 | O   | LYS | A | 309 | 7.281  | 28.420 | -14.539 | 1.00 | 23.42 |
| ATOM | 2358 | N   | LEU | A | 310 | 8.900  | 28.189 | -12.999 | 1.00 | 22.00 |
| ATOM | 2359 | CA  | LEU | A | 310 | 9.906  | 27.866 | -14.002 | 1.00 | 21.73 |
| ATOM | 2360 | CB  | LEU | A | 310 | 11.289 | 28.091 | -13.409 | 1.00 | 21.13 |
| ATOM | 2361 | CG  | LEU | A | 310 | 11.536 | 29.517 | -12.922 | 1.00 | 21.73 |
| ATOM | 2362 | CD1 | LEU | A | 310 | 12.995 | 29.640 | -12.487 | 1.00 | 22.37 |
| ATOM | 2363 | CD2 | LEU | A | 310 | 11.167 | 30.510 | -14.011 | 1.00 | 28.55 |
| ATOM | 2364 | C   | LEU | A | 310 | 9.830  | 26.446 | -14.582 | 1.00 | 21.34 |
| ATOM | 2365 | O   | LEU | A | 310 | 10.478 | 26.145 | -15.598 | 1.00 | 23.36 |
| ATOM | 2366 | N   | ARG | A | 311 | 9.067  | 25.580 | -13.915 | 1.00 | 19.41 |
| ATOM | 2367 | CA  | ARG | A | 311 | 8.862  | 24.211 | -14.373 | 1.00 | 19.13 |
| ATOM | 2368 | CB  | ARG | A | 311 | 9.162  | 23.298 | -13.191 | 1.00 | 20.37 |
| ATOM | 2369 | CG  | ARG | A | 311 | 10.653 | 23.321 | -12.863 | 1.00 | 21.47 |
| ATOM | 2370 | CD  | ARG | A | 311 | 11.008 | 22.805 | -11.476 | 1.00 | 24.25 |
| ATOM | 2371 | NE  | ARG | A | 311 | 10.520 | 21.442 | -11.254 | 1.00 | 23.85 |
| ATOM | 2372 | CZ  | ARG | A | 311 | 10.688 | 20.774 | -10.127 | 1.00 | 22.32 |
| ATOM | 2373 | NH1 | ARG | A | 311 | 11.377 | 21.330 | -9.126  | 1.00 | 25.69 |
| ATOM | 2374 | NH2 | ARG | A | 311 | 10.204 | 19.543 | -9.993  | 1.00 | 18.91 |
| ATOM | 2375 | C   | ARG | A | 311 | 7.431  | 23.931 | -14.838 | 1.00 | 21.21 |
| ATOM | 2376 | O   | ARG | A | 311 | 6.741  | 24.874 | -15.241 | 1.00 | 25.92 |
| ATOM | 2377 | O50 | INH | Z | 1   | 4.605  | 33.376 | 23.736  | 1.00 | 26.83 |
| ATOM | 2378 | C49 | INH | Z | 1   | 4.231  | 34.382 | 24.326  | 1.00 | 26.06 |
| ATOM | 2379 | O51 | INH | Z | 1   | 2.962  | 34.991 | 23.967  | 1.00 | 27.49 |
| ATOM | 2380 | C52 | INH | Z | 1   | 1.903  | 34.307 | 23.285  | 1.00 | 26.93 |
| ATOM | 2381 | C55 | INH | Z | 1   | 0.784  | 35.332 | 23.198  | 1.00 | 23.29 |
| ATOM | 2382 | C54 | INH | Z | 1   | 2.396  | 33.902 | 21.890  | 1.00 | 27.36 |
| ATOM | 2383 | C53 | INH | Z | 1   | 1.427  | 33.119 | 24.127  | 1.00 | 26.28 |
| ATOM | 2384 | N32 | INH | Z | 1   | 4.935  | 34.973 | 25.294  | 1.00 | 24.59 |
| ATOM | 2385 | C31 | INH | Z | 1   | 6.210  | 34.438 | 25.733  | 1.00 | 26.22 |
| ATOM | 2386 | C34 | INH | Z | 1   | 6.924  | 35.626 | 26.369  | 1.00 | 30.49 |
| ATOM | 2387 | C37 | INH | Z | 1   | 7.645  | 36.501 | 25.365  | 1.00 | 33.76 |
| ATOM | 2388 | C39 | INH | Z | 1   | 7.034  | 37.645 | 24.864  | 1.00 | 38.94 |
| ATOM | 2389 | C42 | INH | Z | 1   | 7.713  | 38.450 | 23.950  | 1.00 | 41.70 |
| ATOM | 2390 | C38 | INH | Z | 1   | 9.011  | 38.126 | 23.555  | 1.00 | 44.11 |
| ATOM | 2391 | O47 | INH | Z | 1   | 9.671  | 38.890 | 22.679  | 1.00 | 44.40 |

**FIGURE 298**

|      |      |     |     |   |    |         |        |         |      |       |
|------|------|-----|-----|---|----|---------|--------|---------|------|-------|
| ATOM | 2392 | C41 | INH | Z | 1  | 9.626   | 36.988 | 24.070  | 1.00 | 42.62 |
| ATOM | 2393 | C40 | INH | Z | 1  | 8.945   | 36.181 | 24.978  | 1.00 | 40.44 |
| ATOM | 2394 | C28 | INH | Z | 1  | 5.891   | 33.469 | 26.827  | 1.00 | 26.18 |
| ATOM | 2395 | O30 | INH | Z | 1  | 4.821   | 33.476 | 27.419  | 1.00 | 28.17 |
| ATOM | 2396 | N19 | INH | Z | 1  | 6.822   | 32.576 | 27.106  | 1.00 | 25.35 |
| ATOM | 2397 | C11 | INH | Z | 1  | 6.586   | 31.591 | 28.149  | 1.00 | 22.00 |
| ATOM | 2398 | C20 | INH | Z | 1  | 7.939   | 31.279 | 28.733  | 1.00 | 28.32 |
| ATOM | 2399 | N22 | INH | Z | 1  | 8.016   | 31.042 | 30.046  | 1.00 | 29.86 |
| ATOM | 2400 | C23 | INH | Z | 1  | 9.185   | 30.716 | 30.864  | 1.00 | 32.68 |
| ATOM | 2401 | O21 | INH | Z | 1  | 8.902   | 31.256 | 27.987  | 1.00 | 30.70 |
| ATOM | 2402 | C66 | INH | Z | 1  | 5.982   | 30.345 | 27.471  | 1.00 | 23.98 |
| ATOM | 2403 | C7  | INH | Z | 1  | 6.449   | 29.951 | 26.074  | 1.00 | 24.27 |
| ATOM | 2404 | C4  | INH | Z | 1  | 5.750   | 30.388 | 24.950  | 1.00 | 22.11 |
| ATOM | 2405 | C2  | INH | Z | 1  | 6.147   | 30.039 | 23.651  | 1.00 | 23.96 |
| ATOM | 2406 | C3  | INH | Z | 1  | 7.564   | 29.129 | 25.869  | 1.00 | 22.36 |
| ATOM | 2407 | C6  | INH | Z | 1  | 7.945   | 28.794 | 24.569  | 1.00 | 19.47 |
| ATOM | 2408 | C5  | INH | Z | 1  | 7.273   | 29.237 | 23.440  | 1.00 | 24.64 |
| ATOM | 2409 | N9  | INH | Z | 1  | 7.676   | 28.877 | 22.190  | 1.00 | 20.59 |
| ATOM | 2410 | S14 | INH | Z | 1  | 7.262   | 27.472 | 21.482  | 1.00 | 19.91 |
| ATOM | 2411 | O15 | INH | Z | 1  | 7.837   | 26.333 | 22.230  | 1.00 | 20.79 |
| ATOM | 2412 | O16 | INH | Z | 1  | 7.744   | 27.509 | 20.095  | 1.00 | 20.74 |
| ATOM | 2413 | O17 | INH | Z | 1  | 5.777   | 27.520 | 21.588  | 1.00 | 19.08 |
| ATOM | 2414 | O1  | HOH | W | 1  | -11.455 | 19.036 | 16.241  | 1.00 | 11.20 |
| ATOM | 2415 | O1  | HOH | W | 2  | 10.092  | 17.907 | -7.247  | 1.00 | 15.97 |
| ATOM | 2416 | O1  | HOH | W | 3  | 6.980   | 17.279 | 36.265  | 1.00 | 18.93 |
| ATOM | 2417 | O1  | HOH | W | 4  | 12.344  | 25.665 | -10.547 | 1.00 | 26.47 |
| ATOM | 2418 | O1  | HOH | W | 5  | -0.391  | 18.120 | 30.610  | 1.00 | 15.54 |
| ATOM | 2419 | O1  | HOH | W | 6  | -12.910 | 27.809 | 25.785  | 1.00 | 18.19 |
| ATOM | 2420 | O1  | HOH | W | 7  | 16.795  | 17.314 | 22.020  | 1.00 | 20.81 |
| ATOM | 2421 | O1  | HOH | W | 8  | 10.903  | 18.975 | 31.456  | 1.00 | 19.26 |
| ATOM | 2422 | O1  | HOH | W | 9  | 12.441  | 11.024 | 16.607  | 1.00 | 18.44 |
| ATOM | 2423 | O1  | HOH | W | 10 | -5.476  | 27.892 | 24.187  | 1.00 | 18.18 |
| ATOM | 2424 | O1  | HOH | W | 11 | -5.638  | 29.457 | -12.183 | 1.00 | 22.91 |
| ATOM | 2425 | O1  | HOH | W | 12 | -5.887  | 32.377 | 20.291  | 1.00 | 20.26 |
| ATOM | 2426 | O1  | HOH | W | 13 | 12.670  | 1.352  | 23.922  | 1.00 | 21.55 |
| ATOM | 2427 | O1  | HOH | W | 14 | -2.209  | 18.671 | -7.515  | 1.00 | 17.26 |
| ATOM | 2428 | O1  | HOH | W | 15 | -7.454  | 18.582 | 28.843  | 1.00 | 18.21 |
| ATOM | 2429 | O1  | HOH | W | 16 | -8.860  | 24.488 | 29.900  | 1.00 | 19.86 |
| ATOM | 2430 | O1  | HOH | W | 17 | -2.830  | 35.618 | 3.268   | 1.00 | 21.86 |
| ATOM | 2431 | O1  | HOH | W | 18 | 18.579  | 15.179 | 13.609  | 1.00 | 26.92 |
| ATOM | 2432 | O1  | HOH | W | 19 | -4.688  | 14.506 | 34.209  | 1.00 | 22.07 |
| ATOM | 2433 | O1  | HOH | W | 20 | 2.105   | 17.068 | 26.391  | 1.00 | 16.42 |
| ATOM | 2434 | O1  | HOH | W | 21 | 4.863   | 29.127 | 33.970  | 1.00 | 21.17 |
| ATOM | 2435 | O1  | HOH | W | 22 | -3.568  | 19.852 | 7.077   | 1.00 | 22.18 |
| ATOM | 2436 | O1  | HOH | W | 23 | -5.576  | 3.087  | 15.955  | 1.00 | 26.29 |
| ATOM | 2437 | O1  | HOH | W | 24 | -12.917 | 17.205 | 18.619  | 1.00 | 22.65 |
| ATOM | 2438 | O1  | HOH | W | 25 | 18.698  | 13.470 | 17.368  | 1.00 | 27.43 |
| ATOM | 2439 | O1  | HOH | W | 26 | 1.962   | 17.321 | 29.108  | 1.00 | 20.96 |
| ATOM | 2440 | O1  | HOH | W | 27 | 2.295   | 24.954 | 29.144  | 1.00 | 19.64 |
| ATOM | 2441 | O1  | HOH | W | 28 | -1.602  | 16.134 | 32.029  | 1.00 | 21.50 |
| ATOM | 2442 | O1  | HOH | W | 29 | -0.729  | 38.734 | 15.728  | 1.00 | 29.29 |
| ATOM | 2443 | O1  | HOH | W | 30 | -7.527  | 23.769 | 23.695  | 1.00 | 24.34 |

FIGURE 299

|      |      |    |       |    |         |        |         |      |       |
|------|------|----|-------|----|---------|--------|---------|------|-------|
| ATOM | 2444 | O1 | HOH W | 31 | 14.282  | 22.365 | 16.948  | 1.00 | 22.99 |
| ATOM | 2445 | O1 | HOH W | 32 | -1.604  | 32.781 | -14.649 | 1.00 | 27.92 |
| ATOM | 2446 | O1 | HOH W | 33 | -8.734  | 34.148 | 26.134  | 1.00 | 25.36 |
| ATOM | 2447 | O1 | HOH W | 34 | 8.370   | 30.039 | 18.987  | 1.00 | 21.01 |
| ATOM | 2448 | O1 | HOH W | 35 | 14.794  | 1.864  | 27.548  | 1.00 | 28.16 |
| ATOM | 2449 | O1 | HOH W | 36 | -10.739 | 27.532 | 37.044  | 1.00 | 24.62 |
| ATOM | 2450 | O1 | HOH W | 37 | -7.059  | 1.474  | 21.471  | 1.00 | 25.62 |
| ATOM | 2451 | O1 | HOH W | 38 | -11.234 | 14.555 | 24.148  | 1.00 | 23.76 |
| ATOM | 2452 | O1 | HOH W | 39 | 4.445   | 10.833 | 33.936  | 1.00 | 24.00 |
| ATOM | 2453 | O1 | HOH W | 40 | 7.644   | 22.182 | -5.700  | 1.00 | 31.73 |
| ATOM | 2454 | O1 | HOH W | 41 | -9.581  | 18.385 | 34.798  | 1.00 | 27.77 |
| ATOM | 2455 | O1 | HOH W | 42 | -3.762  | 2.958  | 27.993  | 1.00 | 25.67 |
| ATOM | 2456 | O1 | HOH W | 43 | 16.682  | 28.017 | 20.896  | 1.00 | 27.72 |
| ATOM | 2457 | O1 | HOH W | 44 | 1.889   | 20.014 | 3.611   | 1.00 | 25.02 |
| ATOM | 2458 | O1 | HOH W | 45 | 1.627   | 25.550 | -6.758  | 1.00 | 34.05 |
| ATOM | 2459 | O1 | HOH W | 46 | 0.286   | 7.549  | 9.166   | 1.00 | 38.49 |
| ATOM | 2460 | O1 | HOH W | 47 | -3.896  | 24.915 | 37.139  | 1.00 | 26.95 |
| ATOM | 2461 | O1 | HOH W | 48 | 15.746  | 30.134 | 2.550   | 1.00 | 25.69 |
| ATOM | 2462 | O1 | HOH W | 49 | -5.568  | 10.500 | 33.186  | 1.00 | 28.26 |
| ATOM | 2463 | O1 | HOH W | 50 | -1.650  | 34.023 | 1.496   | 1.00 | 26.31 |
| ATOM | 2464 | O1 | HOH W | 51 | -7.652  | 10.717 | 25.362  | 1.00 | 28.32 |
| ATOM | 2465 | O1 | HOH W | 52 | 0.328   | 0.370  | 13.309  | 1.00 | 27.61 |
| ATOM | 2466 | O1 | HOH W | 53 | 15.355  | 1.106  | 30.215  | 1.00 | 30.33 |
| ATOM | 2467 | O1 | HOH W | 54 | 10.015  | 24.503 | 30.496  | 1.00 | 29.94 |
| ATOM | 2468 | O1 | HOH W | 55 | -11.943 | 35.367 | 17.617  | 1.00 | 28.12 |
| ATOM | 2469 | O1 | HOH W | 56 | -4.357  | -4.311 | 17.098  | 1.00 | 30.10 |
| ATOM | 2470 | O1 | HOH W | 57 | -1.130  | 26.109 | 35.655  | 1.00 | 35.14 |
| ATOM | 2471 | O1 | HOH W | 58 | 6.603   | 33.740 | -5.667  | 1.00 | 34.26 |
| ATOM | 2472 | O1 | HOH W | 59 | -11.191 | 21.716 | 18.000  | 1.00 | 28.53 |
| ATOM | 2473 | O1 | HOH W | 60 | 4.005   | 20.176 | -0.974  | 1.00 | 28.49 |
| ATOM | 2474 | O1 | HOH W | 61 | 15.234  | 25.407 | 33.117  | 1.00 | 33.69 |
| ATOM | 2475 | O1 | HOH W | 62 | 16.720  | 13.787 | 18.961  | 1.00 | 30.06 |
| ATOM | 2476 | O1 | HOH W | 63 | 17.985  | 26.085 | 10.889  | 1.00 | 35.47 |
| ATOM | 2477 | O1 | HOH W | 64 | -4.391  | 35.179 | 19.227  | 1.00 | 26.34 |
| ATOM | 2478 | O1 | HOH W | 65 | -10.126 | 3.407  | 31.678  | 1.00 | 37.24 |
| ATOM | 2479 | O1 | HOH W | 66 | 13.041  | 23.718 | -8.522  | 1.00 | 26.67 |
| ATOM | 2480 | O1 | HOH W | 67 | 15.808  | 27.630 | 0.948   | 1.00 | 31.53 |
| ATOM | 2481 | O1 | HOH W | 68 | -5.194  | 14.828 | 38.851  | 1.00 | 32.15 |
| ATOM | 2482 | O1 | HOH W | 69 | -2.993  | 14.561 | 10.647  | 1.00 | 27.57 |
| ATOM | 2483 | O1 | HOH W | 70 | 4.460   | 25.794 | -13.772 | 1.00 | 29.85 |
| ATOM | 2484 | O1 | HOH W | 71 | -1.043  | 10.807 | 12.546  | 1.00 | 36.09 |
| ATOM | 2485 | O1 | HOH W | 72 | 5.955   | 25.591 | -17.688 | 1.00 | 35.00 |
| ATOM | 2486 | O1 | HOH W | 73 | -4.797  | 23.062 | 3.425   | 1.00 | 23.14 |
| ATOM | 2487 | O1 | HOH W | 74 | 12.930  | 17.207 | 31.823  | 1.00 | 25.65 |
| ATOM | 2488 | O1 | HOH W | 75 | 14.465  | 31.814 | 0.729   | 1.00 | 29.17 |
| ATOM | 2489 | O1 | HOH W | 76 | 11.351  | 8.765  | 29.000  | 1.00 | 29.76 |
| ATOM | 2490 | O1 | HOH W | 77 | -3.463  | 15.346 | 8.038   | 1.00 | 33.01 |
| ATOM | 2491 | O1 | HOH W | 78 | 9.188   | 38.767 | 15.085  | 1.00 | 31.31 |
| ATOM | 2492 | O1 | HOH W | 79 | -2.414  | 9.596  | 32.635  | 1.00 | 44.49 |
| ATOM | 2493 | O1 | HOH W | 80 | -4.993  | 26.536 | 9.601   | 1.00 | 32.37 |
| ATOM | 2494 | O1 | HOH W | 81 | -15.925 | 15.529 | 11.947  | 1.00 | 25.86 |
| ATOM | 2495 | O1 | HOH W | 82 | -12.382 | 18.790 | 35.935  | 1.00 | 34.44 |

**FIGURE 300**



|      |      |    |     |   |     |         |        |        |      |       |
|------|------|----|-----|---|-----|---------|--------|--------|------|-------|
| ATOM | 2496 | O1 | HOH | W | 83  | 2.705   | 48.628 | 10.273 | 1.00 | 40.15 |
| ATOM | 2497 | O1 | HOH | W | 84  | -13.564 | 21.329 | 28.598 | 1.00 | 31.01 |
| ATOM | 2498 | O1 | HOH | W | 85  | 6.479   | 39.636 | 16.774 | 1.00 | 32.83 |
| ATOM | 2499 | O1 | HOH | W | 86  | 14.961  | 4.598  | 28.207 | 1.00 | 29.83 |
| ATOM | 2500 | O1 | HOH | W | 87  | 18.504  | 19.104 | 23.863 | 1.00 | 28.45 |
| ATOM | 2501 | O1 | HOH | W | 88  | 10.773  | 20.142 | -0.695 | 1.00 | 35.21 |
| ATOM | 2502 | O1 | HOH | W | 89  | 3.708   | 16.397 | 0.920  | 1.00 | 38.22 |
| ATOM | 2503 | O1 | HOH | W | 90  | -4.973  | 37.993 | -5.374 | 1.00 | 31.06 |
| ATOM | 2504 | O1 | HOH | W | 91  | 22.103  | 24.540 | 26.314 | 1.00 | 35.14 |
| ATOM | 2505 | O1 | HOH | W | 92  | 10.864  | 34.785 | 14.518 | 1.00 | 48.98 |
| ATOM | 2506 | O1 | HOH | W | 93  | -12.541 | 12.084 | 30.086 | 1.00 | 37.23 |
| ATOM | 2507 | O1 | HOH | W | 94  | 13.549  | -1.341 | 30.361 | 1.00 | 38.12 |
| ATOM | 2508 | O1 | HOH | W | 95  | -3.286  | -3.603 | 24.358 | 1.00 | 30.37 |
| ATOM | 2509 | O1 | HOH | W | 96  | -0.950  | 37.575 | 3.392  | 1.00 | 26.13 |
| ATOM | 2510 | O1 | HOH | W | 97  | 2.862   | 18.800 | 1.412  | 1.00 | 26.47 |
| ATOM | 2511 | O1 | HOH | W | 98  | 2.741   | 4.340  | 11.947 | 1.00 | 42.25 |
| ATOM | 2512 | O1 | HOH | W | 99  | 1.437   | 11.596 | 33.660 | 1.00 | 33.67 |
| ATOM | 2513 | O1 | HOH | W | 100 | -4.898  | 17.123 | 5.233  | 1.00 | 30.59 |
| ATOM | 2514 | O1 | HOH | W | 101 | -0.328  | 39.659 | 22.285 | 1.00 | 37.92 |
| ATOM | 2515 | O1 | HOH | W | 102 | 0.457   | 18.578 | -0.352 | 1.00 | 32.32 |
| ATOM | 2516 | O1 | HOH | W | 103 | 15.238  | 15.465 | 29.462 | 1.00 | 35.78 |
| ATOM | 2517 | O1 | HOH | W | 104 | 12.139  | 22.090 | -0.159 | 1.00 | 34.03 |
| ATOM | 2518 | O1 | HOH | W | 105 | -14.864 | 19.163 | 30.964 | 1.00 | 32.43 |
| ATOM | 2519 | O1 | HOH | W | 106 | -14.505 | 20.555 | 25.186 | 1.00 | 29.82 |
| ATOM | 2520 | O1 | HOH | W | 107 | 3.363   | 34.814 | -7.718 | 1.00 | 34.48 |
| ATOM | 2521 | O1 | HOH | W | 108 | -13.197 | 17.085 | 34.279 | 1.00 | 38.85 |
| ATOM | 2522 | O1 | HOH | W | 109 | -1.443  | 5.382  | 31.117 | 1.00 | 38.54 |
| ATOM | 2523 | O1 | HOH | W | 110 | -0.120  | 14.286 | 35.601 | 1.00 | 31.88 |
| ATOM | 2524 | O1 | HOH | W | 111 | 9.032   | -5.844 | 19.709 | 1.00 | 36.70 |
| ATOM | 2525 | O1 | HOH | W | 112 | 11.379  | 24.876 | -1.986 | 1.00 | 43.81 |
| ATOM | 2526 | O1 | HOH | W | 113 | 12.352  | 38.057 | 2.063  | 1.00 | 31.64 |
| ATOM | 2527 | O1 | HOH | W | 114 | -5.579  | 7.024  | 7.334  | 1.00 | 39.14 |
| ATOM | 2528 | O1 | HOH | W | 115 | -6.985  | 29.910 | -0.433 | 1.00 | 41.07 |
| ATOM | 2529 | O1 | HOH | W | 116 | 5.045   | 33.328 | -8.532 | 1.00 | 37.73 |
| ATOM | 2530 | O1 | HOH | W | 117 | 8.662   | 12.116 | 1.108  | 1.00 | 39.77 |
| ATOM | 2531 | O1 | HOH | W | 118 | -6.293  | 5.912  | 32.542 | 1.00 | 30.14 |
| ATOM | 2532 | O1 | HOH | W | 119 | -13.725 | 11.954 | 27.110 | 1.00 | 39.76 |
| ATOM | 2533 | O1 | HOH | W | 120 | 16.415  | 8.189  | 22.223 | 1.00 | 29.43 |
| ATOM | 2534 | O1 | HOH | W | 121 | -12.645 | 19.481 | 23.348 | 1.00 | 31.08 |
| ATOM | 2535 | O1 | HOH | W | 122 | -13.636 | 39.606 | 9.864  | 1.00 | 39.73 |
| ATOM | 2536 | O1 | HOH | W | 123 | -11.065 | 7.560  | 40.828 | 1.00 | 45.73 |
| ATOM | 2537 | O1 | HOH | W | 124 | -8.777  | 3.390  | 20.560 | 1.00 | 36.17 |
| ATOM | 2538 | O1 | HOH | W | 125 | 3.379   | 22.820 | -2.032 | 1.00 | 27.89 |
| ATOM | 2539 | O1 | HOH | W | 126 | -11.598 | 14.866 | 35.138 | 1.00 | 32.20 |
| ATOM | 2540 | O1 | HOH | W | 127 | -0.940  | 19.672 | 39.788 | 1.00 | 33.34 |
| ATOM | 2541 | O1 | HOH | W | 128 | 15.163  | -4.713 | 22.940 | 1.00 | 36.19 |
| ATOM | 2542 | O1 | HOH | W | 129 | -0.987  | 26.949 | -6.156 | 1.00 | 36.12 |
| ATOM | 2543 | O1 | HOH | W | 130 | 10.863  | 12.854 | 1.718  | 1.00 | 34.61 |
| ATOM | 2544 | O1 | HOH | W | 131 | 14.478  | 36.267 | 1.695  | 1.00 | 41.25 |
| ATOM | 2545 | O1 | HOH | W | 132 | 15.776  | 23.818 | 18.687 | 1.00 | 35.61 |
| ATOM | 2546 | O1 | HOH | W | 133 | 21.161  | 7.231  | 12.795 | 1.00 | 32.15 |
| ATOM | 2547 | O1 | HOH | W | 134 | 22.887  | 22.904 | 29.299 | 1.00 | 36.68 |

FIGURE 301

|      |      |    |           |         |        |         |      |       |
|------|------|----|-----------|---------|--------|---------|------|-------|
| ATOM | 2548 | O1 | HOH W 135 | 3.909   | 17.363 | 36.196  | 1.00 | 35.35 |
| ATOM | 2549 | O1 | HOH W 136 | -12.046 | 11.064 | 22.456  | 1.00 | 35.04 |
| ATOM | 2550 | O1 | HOH W 137 | -12.824 | 27.211 | 19.118  | 1.00 | 38.04 |
| ATOM | 2551 | O1 | HOH W 138 | 14.969  | 31.915 | 7.579   | 1.00 | 35.09 |
| ATOM | 2552 | O1 | HOH W 139 | 13.443  | 32.417 | -3.827  | 1.00 | 44.74 |
| ATOM | 2553 | O1 | HOH W 140 | 2.776   | 12.732 | 37.520  | 1.00 | 41.66 |
| ATOM | 2554 | O1 | HOH W 141 | -1.350  | 12.666 | 37.266  | 1.00 | 40.38 |
| ATOM | 2555 | O1 | HOH W 142 | 3.324   | 6.477  | 10.524  | 1.00 | 37.22 |
| ATOM | 2556 | O1 | HOH W 143 | -16.166 | 29.270 | 31.100  | 1.00 | 36.51 |
| ATOM | 2557 | O1 | HOH W 144 | 16.001  | -2.359 | 30.645  | 1.00 | 44.06 |
| ATOM | 2558 | O1 | HOH W 145 | 2.861   | 45.550 | 14.180  | 1.00 | 45.63 |
| ATOM | 2559 | O1 | HOH W 146 | 4.593   | 25.045 | 35.681  | 1.00 | 44.05 |
| ATOM | 2560 | O1 | HOH W 147 | -5.762  | 3.453  | 30.636  | 1.00 | 34.95 |
| ATOM | 2561 | O1 | HOH W 148 | -8.031  | 24.355 | 12.086  | 1.00 | 35.62 |
| ATOM | 2562 | O1 | HOH W 149 | -6.652  | 22.984 | -0.071  | 1.00 | 31.34 |
| ATOM | 2563 | O1 | HOH W 150 | -9.852  | 26.486 | 11.576  | 1.00 | 53.30 |
| ATOM | 2564 | O1 | HOH W 151 | -11.032 | 13.045 | 39.495  | 1.00 | 41.67 |
| ATOM | 2565 | O1 | HOH W 152 | -5.662  | -6.734 | 17.860  | 1.00 | 50.02 |
| ATOM | 2566 | O1 | HOH W 153 | -14.654 | 10.777 | 19.722  | 1.00 | 39.18 |
| ATOM | 2567 | O1 | HOH W 154 | 11.452  | 35.739 | 9.234   | 1.00 | 31.71 |
| ATOM | 2568 | O1 | HOH W 155 | -0.977  | 7.991  | -0.542  | 1.00 | 45.59 |
| ATOM | 2569 | O1 | HOH W 156 | 11.447  | 44.304 | 4.341   | 1.00 | 42.42 |
| ATOM | 2570 | O1 | HOH W 157 | 20.425  | 25.089 | 10.825  | 1.00 | 38.33 |
| ATOM | 2571 | O1 | HOH W 158 | -0.478  | 42.056 | 23.691  | 1.00 | 40.14 |
| ATOM | 2572 | O1 | HOH W 159 | -13.365 | 36.694 | 5.529   | 1.00 | 49.14 |
| ATOM | 2573 | O1 | HOH W 160 | 15.601  | 29.777 | 23.845  | 1.00 | 36.82 |
| ATOM | 2574 | O1 | HOH W 161 | 10.807  | 30.311 | 34.040  | 1.00 | 40.96 |
| ATOM | 2575 | O1 | HOH W 162 | -4.239  | 12.123 | 10.131  | 1.00 | 32.53 |
| ATOM | 2576 | O1 | HOH W 163 | -15.155 | 30.501 | 26.593  | 1.00 | 34.26 |
| ATOM | 2577 | O1 | HOH W 164 | 17.868  | 18.293 | 5.518   | 1.00 | 38.35 |
| ATOM | 2578 | O1 | HOH W 165 | -3.791  | 2.469  | 10.886  | 1.00 | 39.48 |
| ATOM | 2579 | O1 | HOH W 166 | -13.791 | 14.215 | 31.432  | 1.00 | 38.00 |
| ATOM | 2580 | O1 | HOH W 167 | 0.432   | 17.497 | 39.137  | 1.00 | 42.73 |
| ATOM | 2581 | O1 | HOH W 168 | -17.968 | 15.461 | 15.749  | 1.00 | 41.59 |
| ATOM | 2582 | O1 | HOH W 169 | 3.057   | 38.735 | -8.809  | 1.00 | 36.15 |
| ATOM | 2583 | O1 | HOH W 170 | -13.284 | 32.522 | 19.061  | 1.00 | 43.72 |
| ATOM | 2584 | O1 | HOH W 171 | 9.161   | 39.858 | 11.511  | 1.00 | 61.20 |
| ATOM | 2585 | O1 | HOH W 172 | -8.076  | 25.214 | 1.277   | 1.00 | 34.46 |
| ATOM | 2586 | O1 | HOH W 173 | 2.413   | -7.723 | 17.535  | 1.00 | 50.89 |
| ATOM | 2587 | O1 | HOH W 174 | 7.967   | 38.224 | -3.285  | 1.00 | 35.96 |
| ATOM | 2588 | O1 | HOH W 175 | 10.930  | 20.638 | 33.730  | 1.00 | 35.38 |
| ATOM | 2589 | O1 | HOH W 176 | 4.602   | 2.675  | 11.036  | 1.00 | 36.17 |
| ATOM | 2590 | O1 | HOH W 177 | 4.229   | 47.562 | 3.051   | 1.00 | 39.90 |
| ATOM | 2591 | O1 | HOH W 178 | 15.151  | 17.822 | 29.427  | 1.00 | 40.53 |
| ATOM | 2592 | O1 | HOH W 179 | -1.974  | 45.545 | 5.497   | 1.00 | 42.30 |
| ATOM | 2593 | O1 | HOH W 180 | -11.790 | 5.702  | 19.435  | 1.00 | 46.01 |
| ATOM | 2594 | O1 | HOH W 181 | -3.116  | 46.090 | 12.430  | 1.00 | 36.56 |
| ATOM | 2595 | O1 | HOH W 182 | -2.855  | 17.252 | -3.365  | 1.00 | 46.55 |
| ATOM | 2596 | O1 | HOH W 183 | 16.937  | 14.782 | 22.299  | 1.00 | 45.85 |
| ATOM | 2597 | O1 | HOH W 184 | 15.864  | 28.547 | 32.612  | 1.00 | 52.60 |
| ATOM | 2598 | O1 | HOH W 185 | -12.223 | 41.151 | 11.021  | 1.00 | 46.56 |
| ATOM | 2599 | O1 | HOH W 186 | -3.669  | 35.551 | -11.268 | 1.00 | 45.80 |

**FIGURE 302**

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Three Dimensional Coordinates of HPTPbeta

|      |      |    |           |         |        |         |      |       |
|------|------|----|-----------|---------|--------|---------|------|-------|
| ATOM | 2600 | O1 | HOH W 187 | -13.450 | 16.205 | 23.864  | 1.00 | 39.99 |
| ATOM | 2601 | O1 | HOH W 188 | 21.557  | 8.538  | 9.074   | 1.00 | 32.39 |
| ATOM | 2602 | O1 | HOH W 189 | 1.733   | 29.325 | -10.520 | 1.00 | 44.58 |
| ATOM | 2603 | O1 | HOH W 190 | -1.094  | 24.213 | 42.979  | 1.00 | 44.98 |
| ATOM | 2604 | O1 | HOH W 191 | -6.827  | 4.971  | 4.805   | 1.00 | 47.90 |
| ATOM | 2605 | O1 | HOH W 192 | -13.991 | 33.731 | 13.221  | 1.00 | 40.59 |
| ATOM | 2606 | O1 | HOH W 193 | 13.588  | 13.644 | -1.450  | 1.00 | 40.18 |
| ATOM | 2607 | O1 | HOH W 194 | -5.326  | 32.039 | -9.354  | 1.00 | 38.33 |
| ATOM | 2608 | O1 | HOH W 195 | 13.465  | 33.762 | -13.581 | 1.00 | 39.35 |
| ATOM | 2609 | O1 | HOH W 196 | 20.141  | -1.476 | 26.767  | 1.00 | 58.47 |
| ATOM | 2610 | O1 | HOH W 197 | -13.105 | 19.480 | 20.652  | 1.00 | 48.59 |
| ATOM | 2611 | O1 | HOH W 198 | 7.070   | 7.353  | 33.532  | 1.00 | 49.27 |
| ATOM | 2612 | O1 | HOH W 199 | 6.799   | 28.923 | -16.944 | 1.00 | 51.04 |
| ATOM | 2613 | O1 | HOH W 200 | 0.389   | 6.026  | 29.372  | 1.00 | 35.03 |
| ATOM | 2614 | O1 | HOH W 201 | 8.386   | 25.655 | 32.893  | 1.00 | 37.20 |
| ATOM | 2615 | O1 | HOH W 202 | 17.615  | -0.073 | 29.521  | 1.00 | 48.46 |
| ATOM | 2616 | O1 | HOH W 203 | -6.124  | 28.880 | 4.959   | 1.00 | 35.61 |
| ATOM | 2617 | O1 | HOH W 204 | 13.941  | 6.496  | 29.759  | 1.00 | 53.62 |
| ATOM | 2618 | O1 | HOH W 205 | 16.954  | -0.234 | 14.375  | 1.00 | 37.68 |
| ATOM | 2619 | O1 | HOH W 206 | 2.522   | -7.489 | 20.961  | 1.00 | 44.59 |
| ATOM | 2620 | O1 | HOH W 207 | 5.703   | 49.354 | 10.543  | 1.00 | 44.22 |
| ATOM | 2621 | O1 | HOH W 208 | -9.111  | 38.567 | 12.389  | 1.00 | 50.27 |
| ATOM | 2622 | O1 | HOH W 209 | -7.236  | 20.258 | 6.492   | 1.00 | 35.19 |
| ATOM | 2623 | O1 | HOH W 210 | 8.786   | 5.463  | 31.949  | 1.00 | 35.74 |
| ATOM | 2624 | O1 | HOH W 211 | -7.222  | 40.672 | 16.386  | 1.00 | 42.49 |
| ATOM | 2625 | O1 | HOH W 212 | 12.825  | 34.503 | 7.617   | 1.00 | 38.94 |
| ATOM | 2626 | O1 | HOH W 213 | 5.590   | 30.888 | 31.645  | 1.00 | 26.09 |
| ATOM | 2627 | O1 | HOH W 214 | 9.169   | 32.503 | 25.209  | 1.00 | 41.71 |
| ATOM | 2628 | O1 | HOH W 215 | 23.574  | 26.554 | 10.071  | 1.00 | 56.57 |
| ATOM | 2629 | O1 | HOH W 216 | 10.056  | 38.516 | -1.760  | 1.00 | 38.36 |
| ATOM | 2630 | O1 | HOH W 217 | -5.653  | 23.538 | 10.071  | 1.00 | 39.02 |
| ATOM | 2631 | O1 | HOH W 218 | -9.772  | 39.888 | 16.597  | 1.00 | 39.89 |
| ATOM | 2632 | O1 | HOH W 219 | -7.677  | 22.937 | 7.244   | 1.00 | 48.50 |
| ATOM | 2633 | O1 | HOH W 220 | -8.099  | 10.871 | 39.914  | 1.00 | 44.93 |
| ATOM | 2634 | O1 | HOH W 221 | 9.902   | 31.834 | 22.653  | 1.00 | 46.40 |
| ATOM | 2635 | O1 | HOH W 222 | 3.536   | 38.208 | 17.936  | 1.00 | 39.89 |
| ATOM | 2636 | O1 | HOH W 223 | 5.427   | 12.563 | -2.175  | 1.00 | 43.37 |
| ATOM | 2637 | O1 | HOH W 224 | 19.901  | 17.833 | 4.495   | 1.00 | 39.94 |
| ATOM | 2638 | O1 | HOH W 225 | -12.027 | 36.815 | 13.817  | 1.00 | 44.07 |
| ATOM | 2639 | O1 | HOH W 226 | -8.746  | 32.585 | 28.696  | 1.00 | 48.46 |
| ATOM | 2640 | O1 | HOH W 227 | 17.914  | 15.042 | 24.333  | 1.00 | 48.17 |
| ATOM | 2641 | O1 | HOH W 228 | -15.428 | 28.994 | 22.176  | 1.00 | 32.12 |
| ATOM | 2642 | O1 | HOH W 229 | -1.184  | 15.555 | 39.910  | 1.00 | 42.24 |
| ATOM | 2643 | O1 | HOH W 230 | 1.784   | 16.997 | 9.532   | 1.00 | 38.28 |
| ATOM | 2644 | O1 | HOH W 231 | -4.431  | 5.259  | 30.630  | 1.00 | 57.46 |
| ATOM | 2645 | O1 | HOH W 232 | 14.418  | 34.885 | 17.296  | 1.00 | 49.40 |
| ATOM | 2646 | O1 | HOH W 233 | -10.428 | 31.639 | 7.906   | 1.00 | 38.03 |
| ATOM | 2647 | O1 | HOH W 234 | 21.073  | 3.624  | 22.298  | 1.00 | 46.76 |
| ATOM | 2648 | O1 | HOH W 235 | 9.325   | 20.879 | -6.720  | 1.00 | 46.19 |
| ATOM | 2649 | O1 | HOH W 236 | 10.266  | 24.192 | -17.765 | 1.00 | 43.43 |
| ATOM | 2650 | O1 | HOH W 237 | 2.085   | -3.234 | 15.986  | 1.00 | 49.75 |
| ATOM | 2651 | O1 | HOH W 238 | -0.063  | 5.328  | 10.360  | 1.00 | 52.94 |

**FIGURE 303**

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|      |      |    |           |         |        |         |      |       |
|------|------|----|-----------|---------|--------|---------|------|-------|
| ATOM | 2652 | O1 | HOH W 239 | 10.028  | 22.924 | 33.652  | 1.00 | 45.99 |
| ATOM | 2653 | O1 | HOH W 240 | 16.681  | 32.926 | 16.387  | 1.00 | 43.29 |
| ATOM | 2654 | O1 | HOH W 241 | 7.871   | 13.034 | 37.758  | 1.00 | 46.97 |
| ATOM | 2655 | O1 | HOH W 242 | -7.500  | 33.136 | -10.047 | 1.00 | 53.39 |
| ATOM | 2656 | O1 | HOH W 243 | 20.580  | 20.554 | 3.052   | 1.00 | 48.18 |
| ATOM | 2657 | O1 | HOH W 244 | 17.540  | 25.077 | 8.214   | 1.00 | 43.50 |
| ATOM | 2658 | O1 | HOH W 245 | -5.445  | 39.439 | 24.106  | 1.00 | 43.55 |
| ATOM | 2659 | O1 | HOH W 246 | 10.166  | 40.681 | 14.159  | 1.00 | 41.16 |
| ATOM | 2660 | O1 | HOH W 247 | 19.127  | 23.993 | 6.155   | 1.00 | 40.29 |
| ATOM | 2661 | O1 | HOH W 248 | -5.962  | 35.247 | -11.325 | 1.00 | 64.60 |
| ATOM | 2662 | O1 | HOH W 249 | -13.021 | 14.668 | 4.628   | 1.00 | 58.02 |
| ATOM | 2663 | O1 | HOH W 250 | -15.666 | 12.941 | 32.852  | 1.00 | 45.95 |
| ATOM | 2664 | O1 | HOH W 251 | -5.827  | 4.361  | 28.098  | 1.00 | 39.00 |
| ATOM | 2665 | O1 | HOH W 252 | -4.508  | 4.229  | 4.028   | 1.00 | 58.76 |
| ATOM | 2666 | O1 | HOH W 253 | -1.679  | 36.793 | -11.023 | 1.00 | 54.88 |
| ATOM | 2667 | O1 | HOH W 254 | -3.188  | 12.850 | 35.709  | 1.00 | 44.15 |
| ATOM | 2668 | O1 | HOH W 255 | -4.863  | 46.499 | 9.267   | 1.00 | 47.64 |
| ATOM | 2669 | O1 | HOH W 256 | -8.876  | 14.076 | 39.968  | 1.00 | 49.77 |
| ATOM | 2670 | O1 | HOH W 257 | -7.413  | 15.403 | 42.092  | 1.00 | 56.43 |
| ATOM | 2671 | O1 | HOH W 258 | 15.526  | 32.542 | 13.982  | 1.00 | 38.82 |
| ATOM | 2672 | O1 | HOH W 259 | 16.627  | 29.755 | 30.106  | 1.00 | 59.92 |
| ATOM | 2673 | O1 | HOH W 260 | -6.350  | 21.495 | 10.220  | 1.00 | 44.14 |
| ATOM | 2674 | O1 | HOH W 261 | -10.475 | 11.052 | 40.121  | 1.00 | 46.63 |
| ATOM | 2675 | O1 | HOH W 262 | -16.169 | 28.237 | 33.252  | 1.00 | 50.35 |
| ATOM | 2676 | O1 | HOH W 263 | 21.143  | 26.244 | 7.273   | 1.00 | 49.50 |
| ATOM | 2677 | O1 | HOH W 264 | 18.544  | 3.658  | 19.522  | 1.00 | 54.96 |
| ATOM | 2678 | O1 | HOH W 265 | -13.057 | 36.485 | 10.921  | 1.00 | 57.92 |
| ATOM | 2679 | O1 | HOH W 266 | -14.213 | 30.872 | 7.965   | 1.00 | 55.62 |
| ATOM | 2680 | O1 | HOH W 267 | 23.105  | 19.120 | 9.667   | 1.00 | 51.70 |
| ATOM | 2681 | O1 | HOH W 268 | 19.557  | 23.525 | 21.545  | 1.00 | 55.10 |
| ATOM | 2682 | O1 | HOH W 269 | -6.887  | 8.335  | 40.062  | 1.00 | 53.82 |
| ATOM | 2683 | O1 | HOH W 270 | 12.547  | 34.227 | 22.521  | 1.00 | 60.24 |
| ATOM | 2684 | O1 | HOH W 271 | -3.101  | -0.406 | 15.411  | 1.00 | 43.16 |
| ATOM | 2685 | O1 | HOH W 272 | 2.686   | 50.220 | 2.020   | 1.00 | 56.09 |
| ATOM | 2686 | O1 | HOH W 273 | -14.257 | 29.391 | 17.420  | 1.00 | 56.26 |
| ATOM | 2687 | O1 | HOH W 274 | -7.269  | 25.617 | 22.970  | 1.00 | 58.39 |
| ATOM | 2688 | O1 | HOH W 275 | -2.828  | 0.486  | 9.670   | 1.00 | 60.53 |
| ATOM | 2689 | O1 | HOH W 276 | 9.879   | 32.192 | -10.785 | 1.00 | 50.33 |
| ATOM | 2690 | O1 | HOH W 277 | -13.291 | 27.301 | 37.675  | 1.00 | 47.65 |
| ATOM | 2691 | O1 | HOH W 278 | 9.031   | 40.412 | -7.375  | 1.00 | 59.24 |
| ATOM | 2692 | O1 | HOH W 279 | 21.333  | 22.702 | 9.534   | 1.00 | 50.34 |
| ATOM | 2693 | O1 | HOH W 280 | 10.062  | 2.181  | 11.069  | 1.00 | 63.85 |
| ATOM | 2694 | O1 | HOH W 281 | -11.670 | 11.608 | 25.465  | 1.00 | 48.90 |
| ATOM | 2695 | O1 | HOH W 282 | 5.882   | 36.123 | 22.042  | 1.00 | 58.95 |
| ATOM | 2696 | O1 | HOH W 283 | -4.121  | 5.854  | 34.338  | 1.00 | 54.24 |
| ATOM | 2697 | O1 | HOH W 284 | -9.020  | 5.421  | 40.050  | 1.00 | 56.11 |
| END  |      |    |           |         |        |         |      |       |

**FIGURE 304**